EFRC
Energy Frontier Research Center
for gas separations relevant to clean air technologies

ENERGY FRONTIER RESEARCH CENTER

for gas separations relevant to clean air technologie

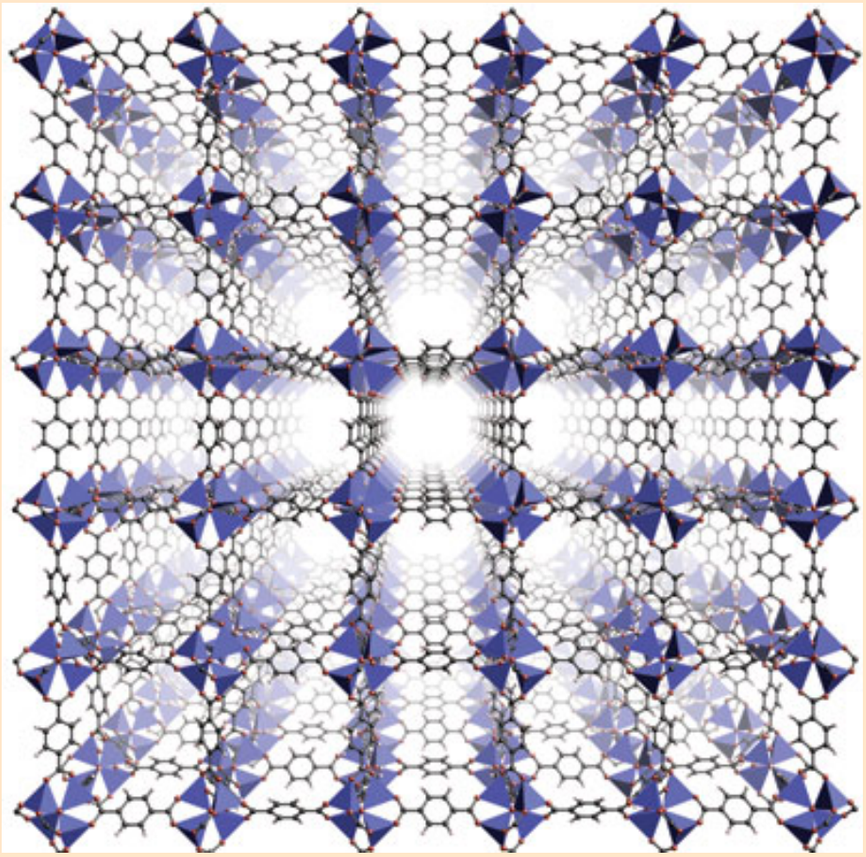
new materials for capture...

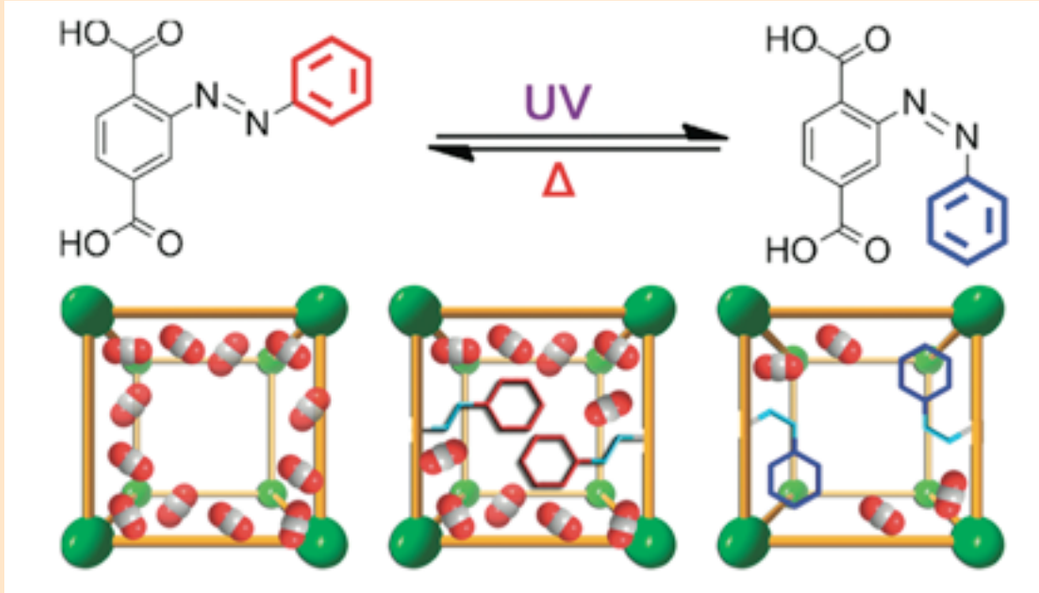
new methods to characterize...

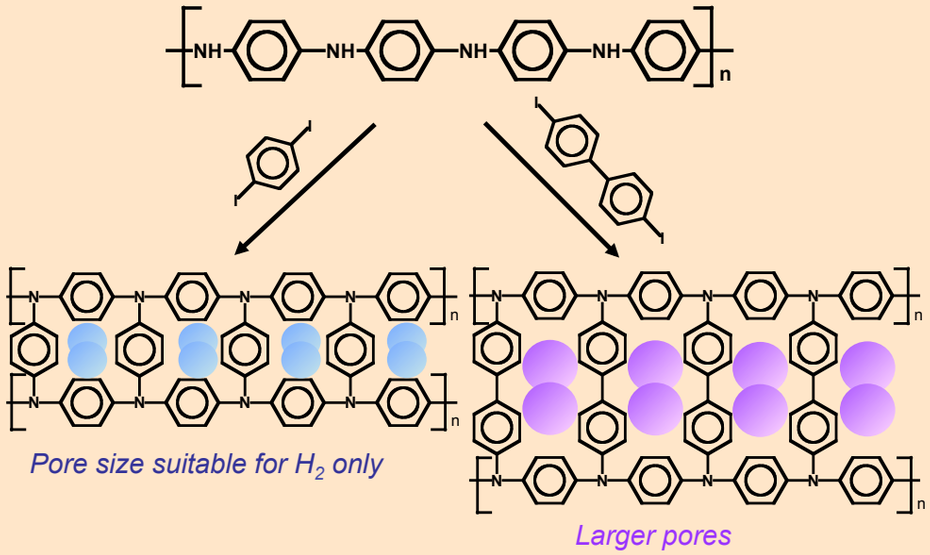
new ways to compute...

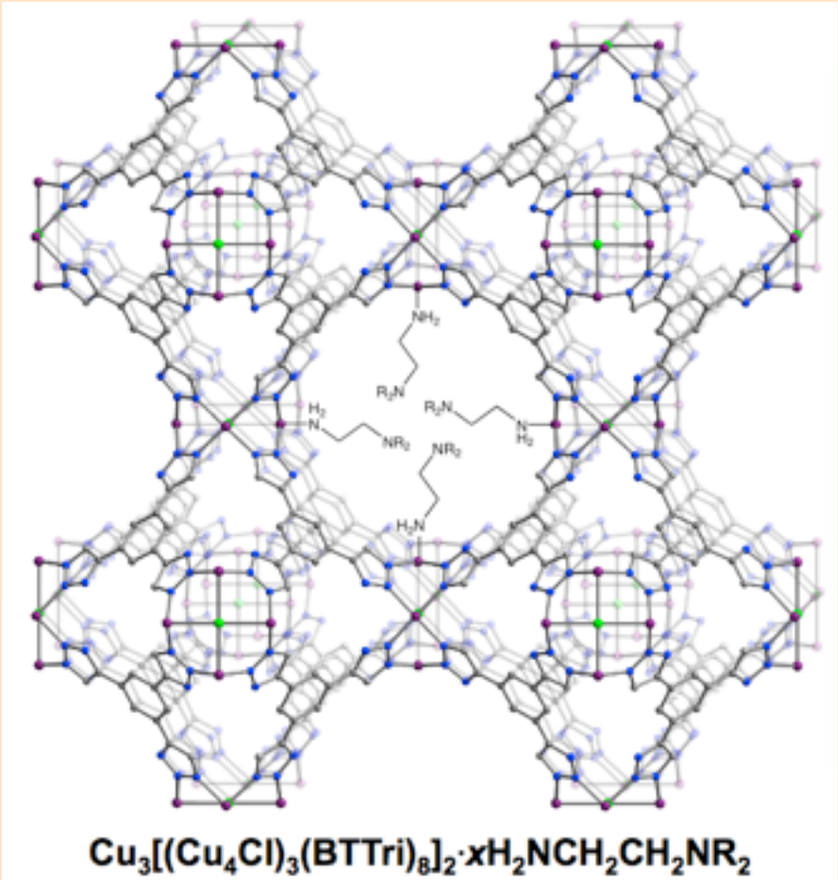
new ways to communicate...

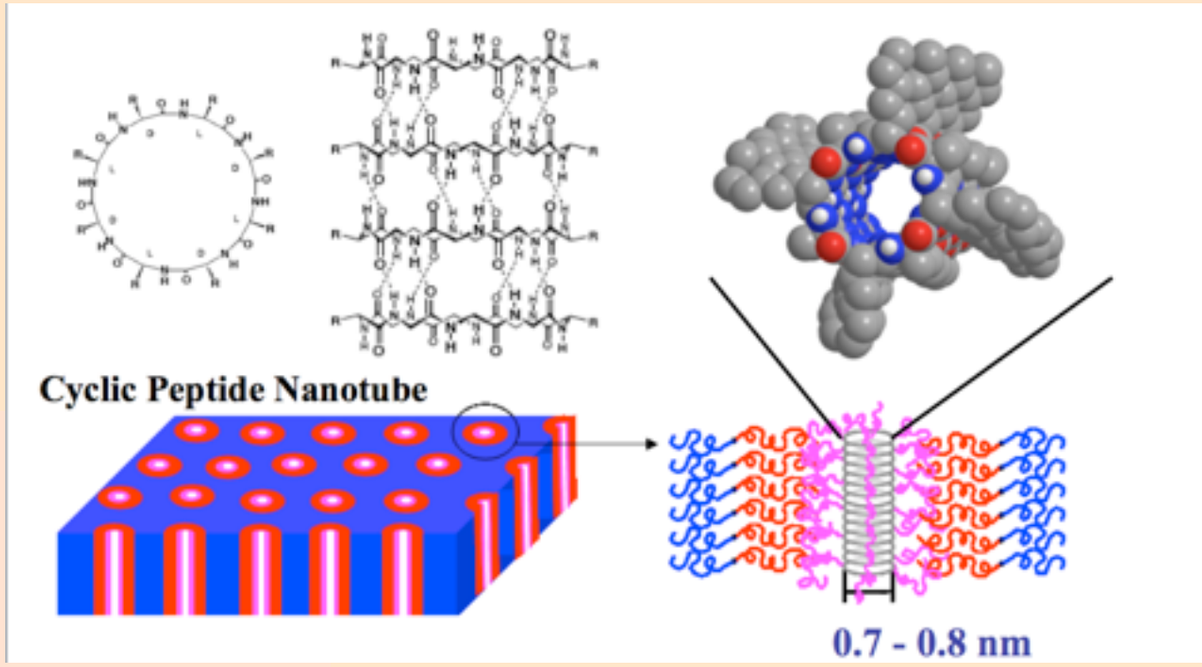
new materials for capture...



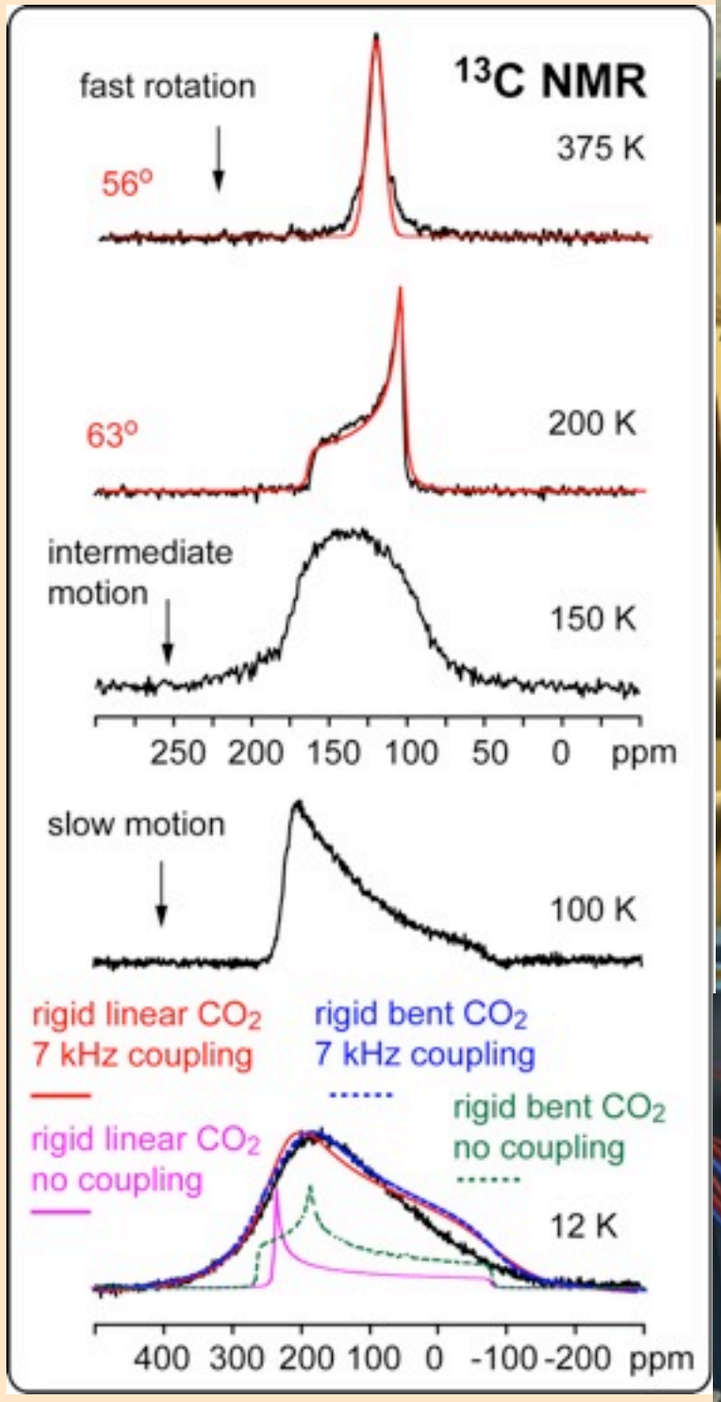


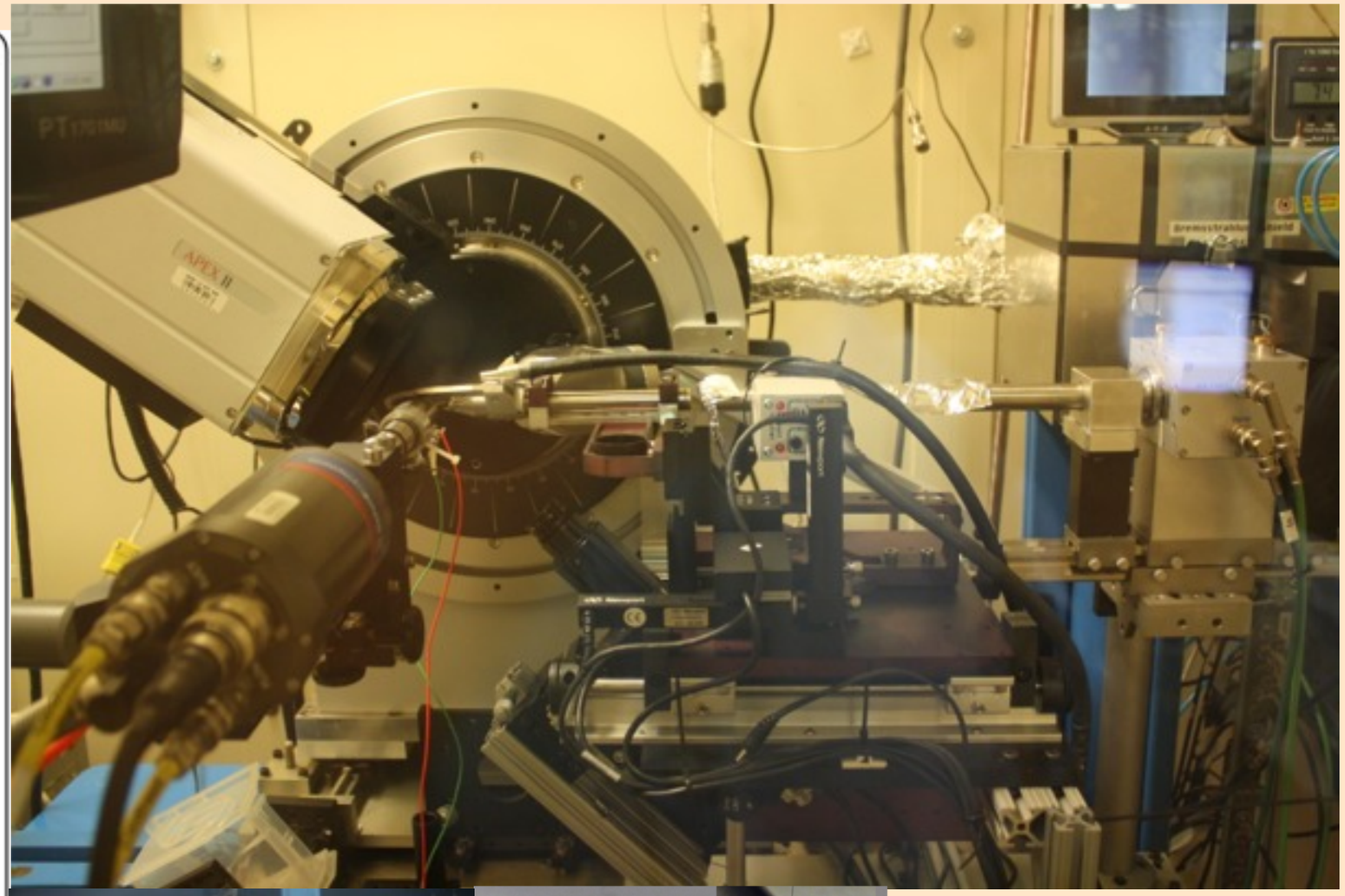


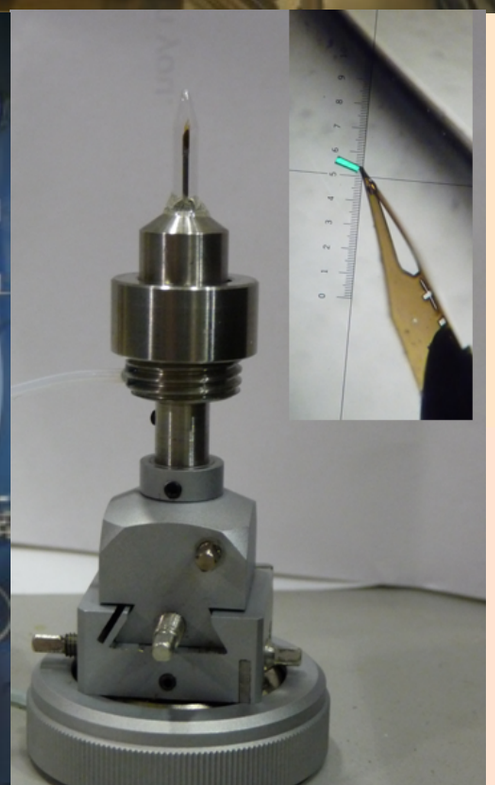




new methods to characterize...







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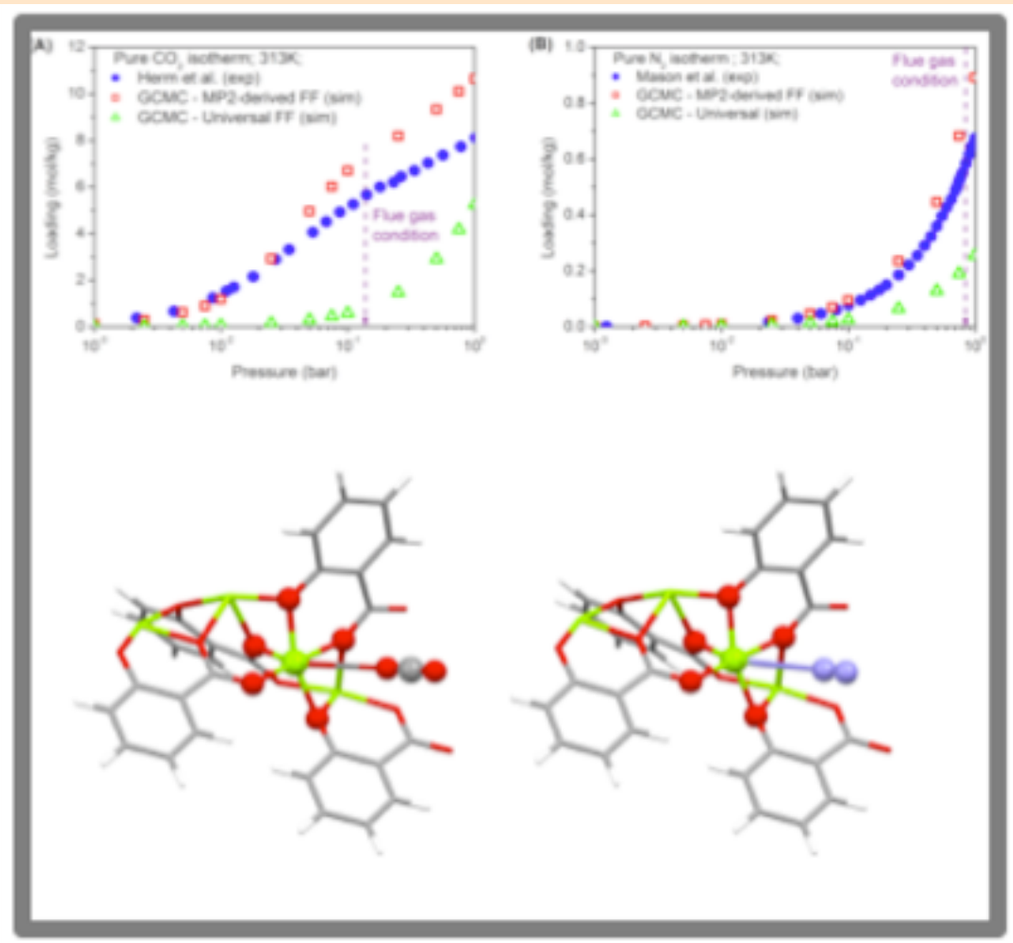
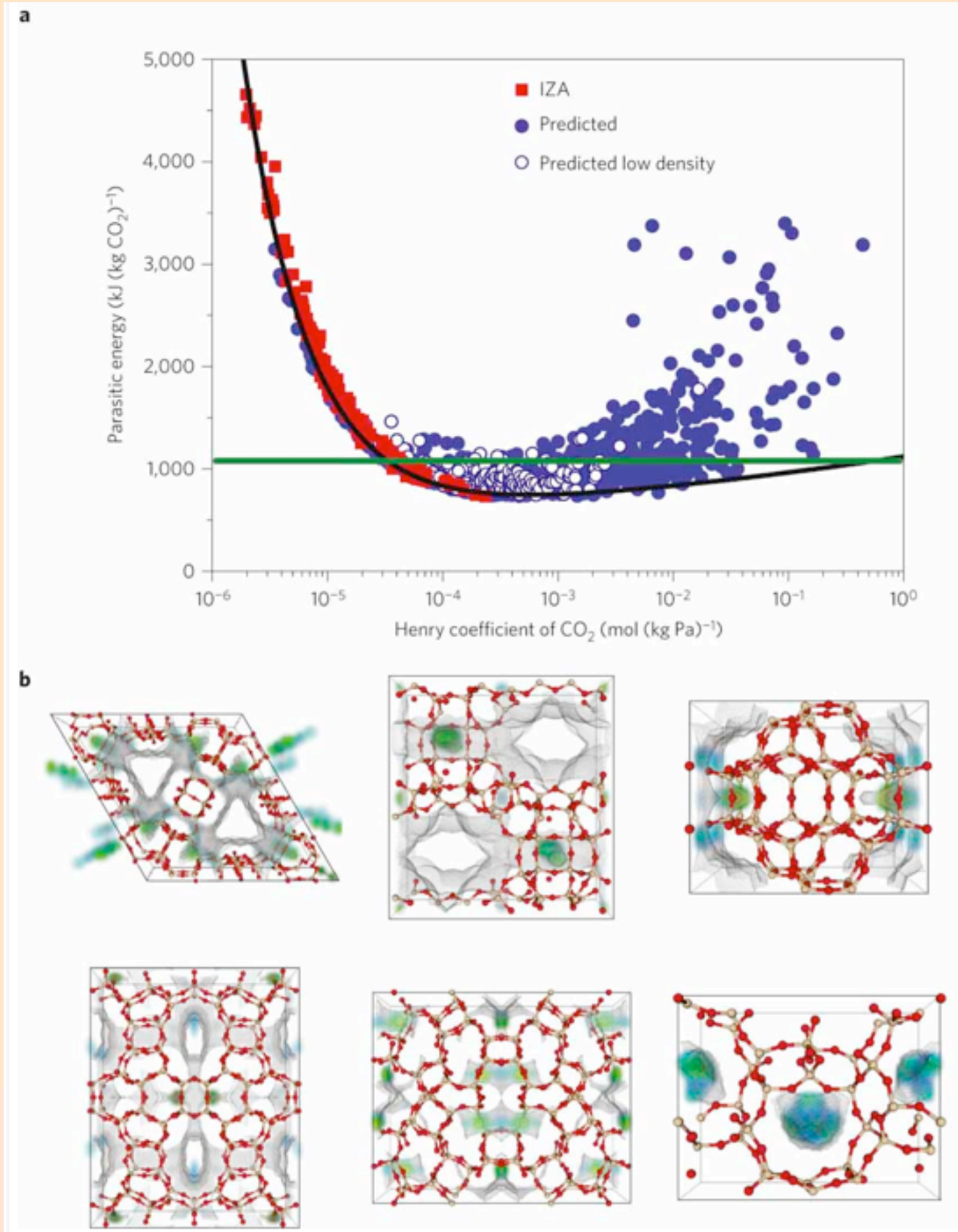
new ways to compute...





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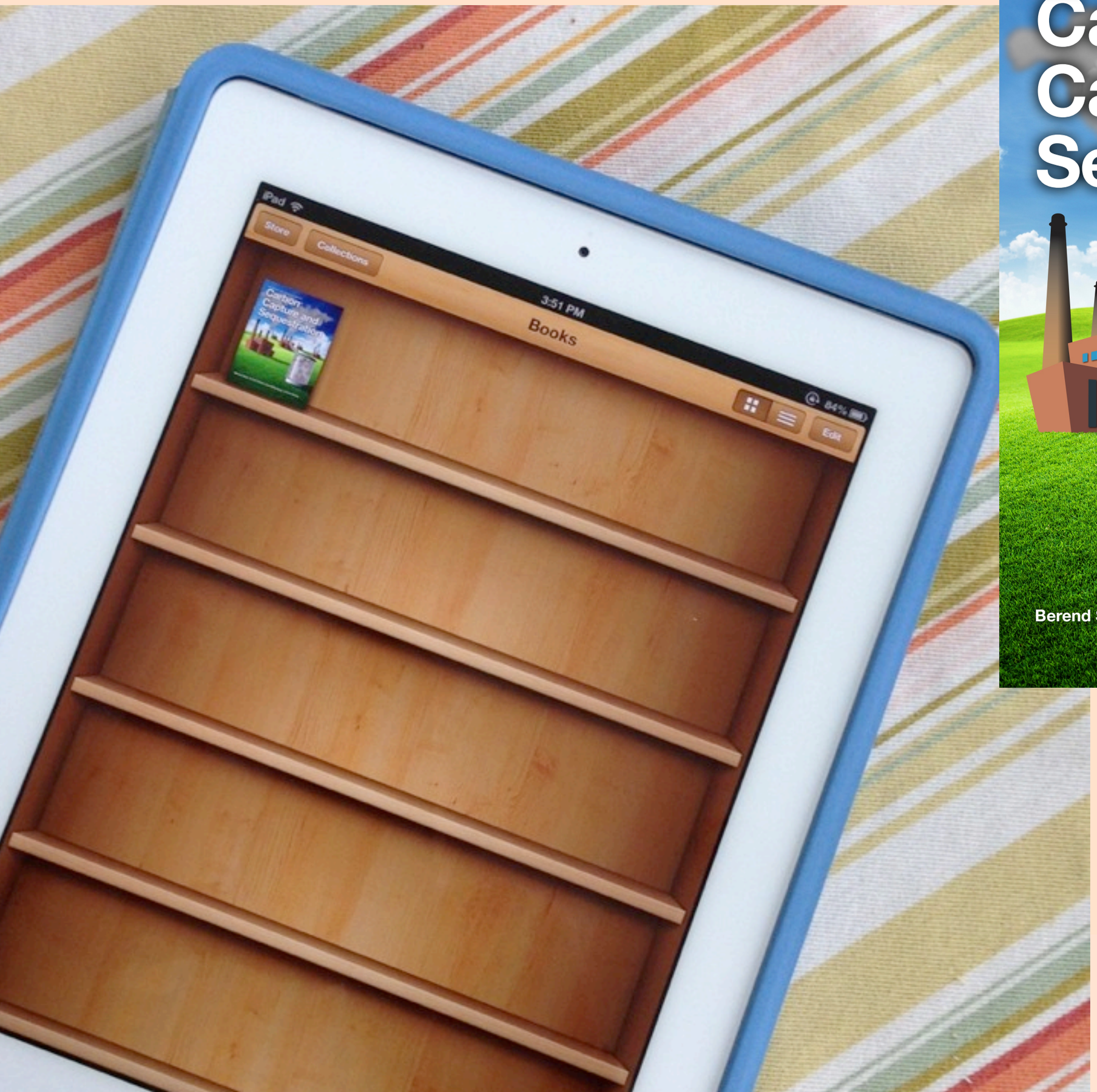
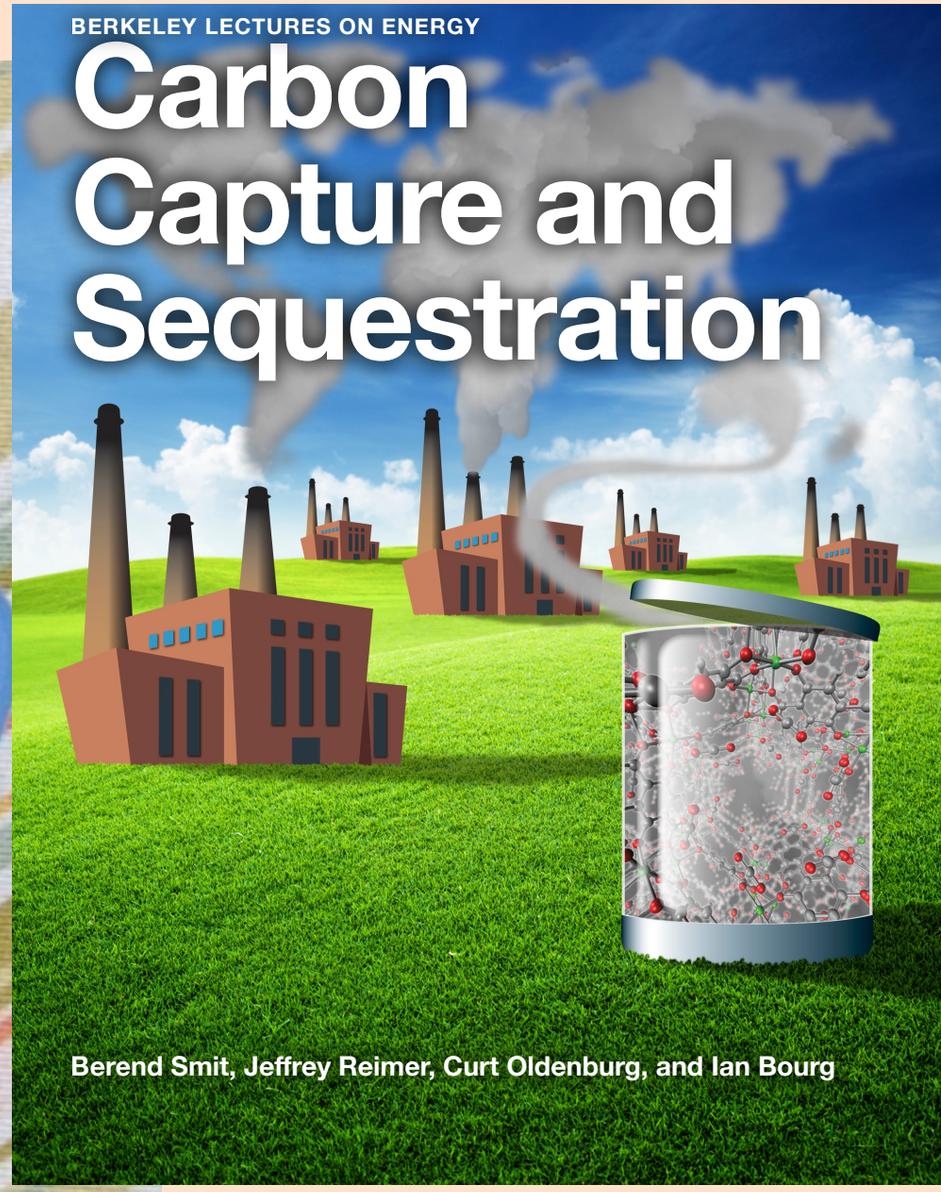
new ways to communicate...





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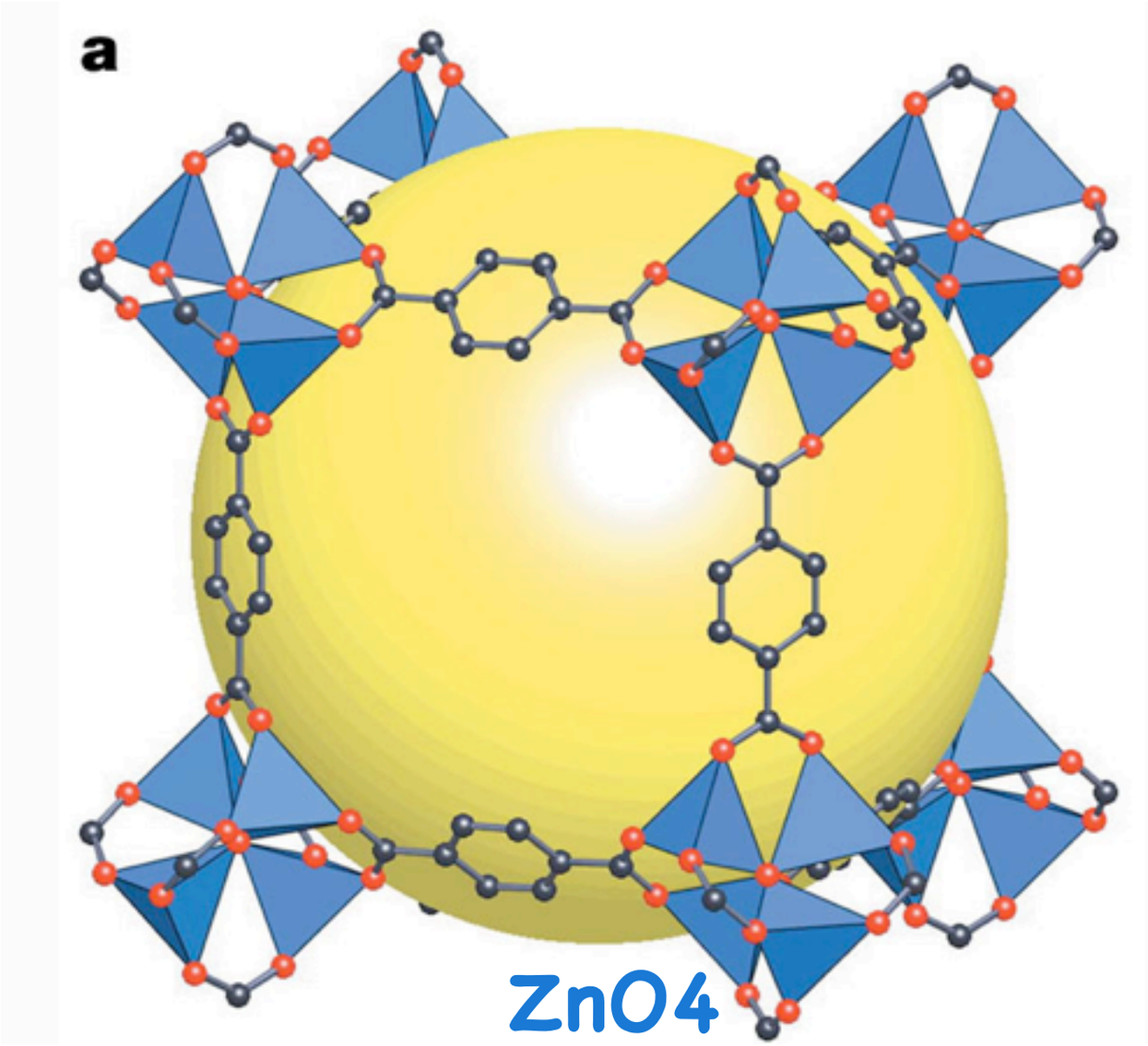
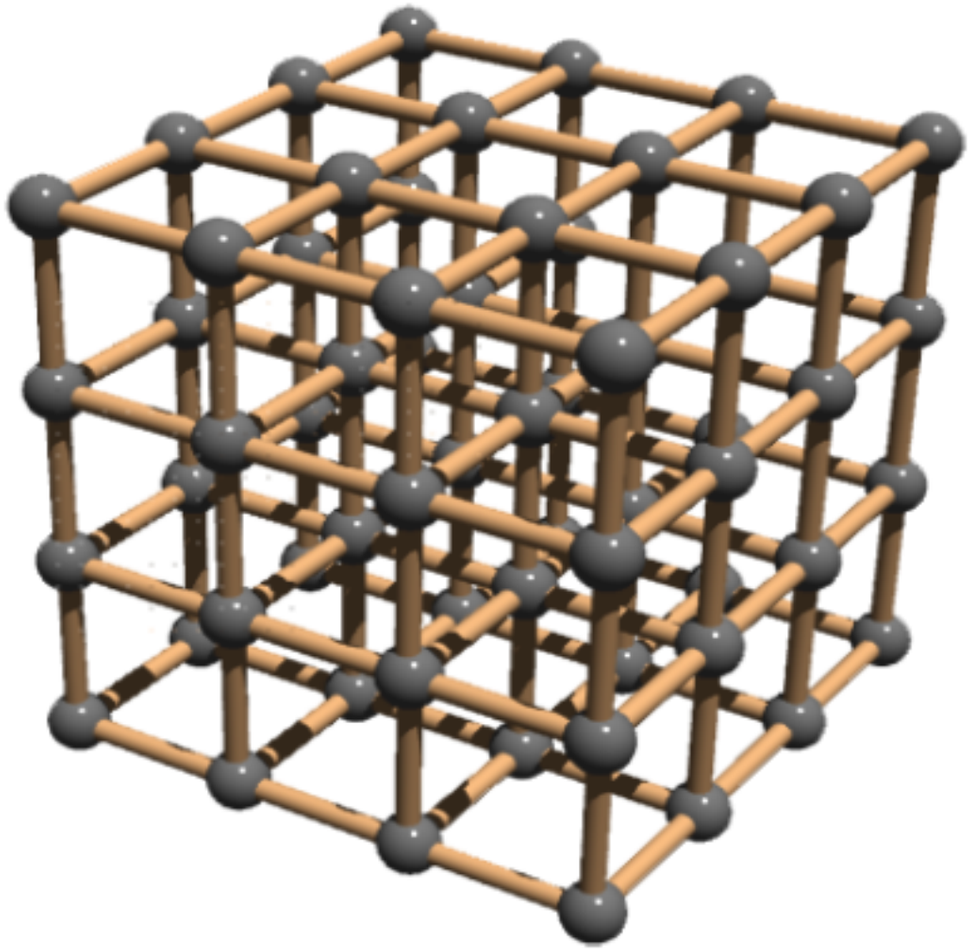
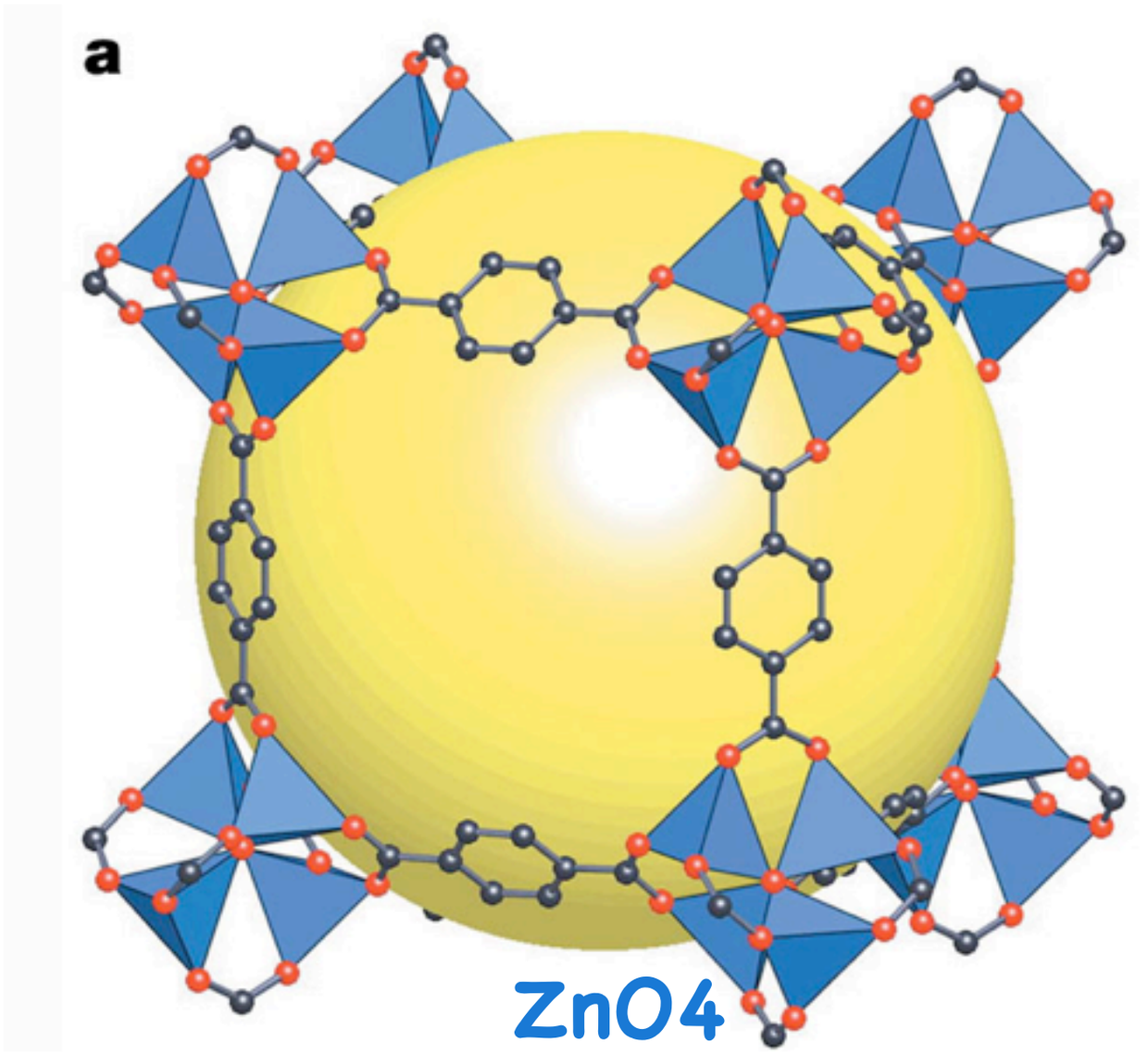
"MOF-5"



ZnO4
tetrahedra



"MOF-5"



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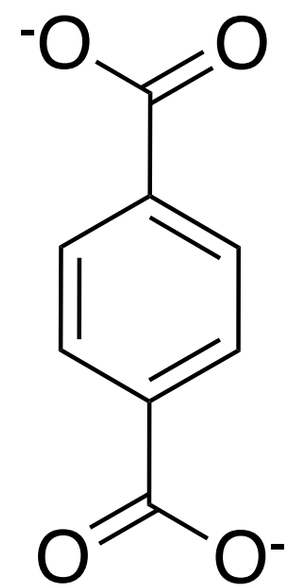
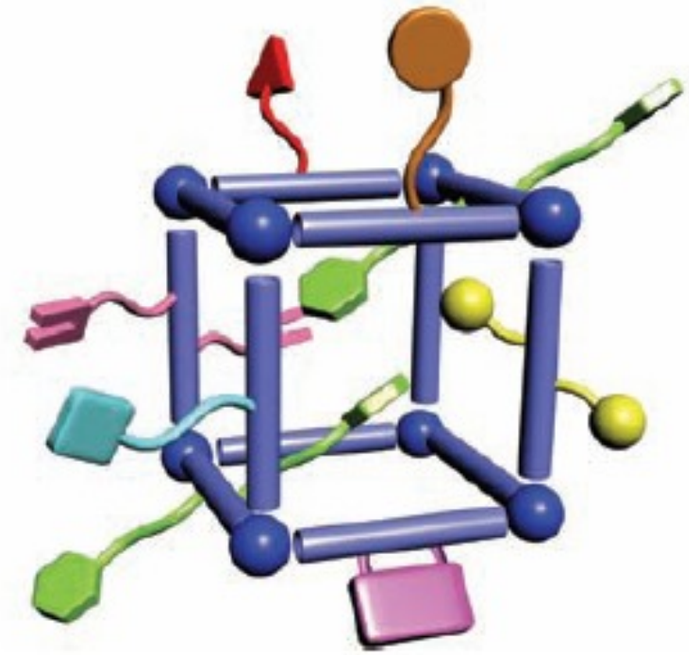


organic linker

Prof. Omar Yaghi
LBNL and Dept. of
Chemistry, UCB

MTV-MOFs: MOFs with multivariate organic linkers



MTV-MOF-5 structure
with eight different functionalities

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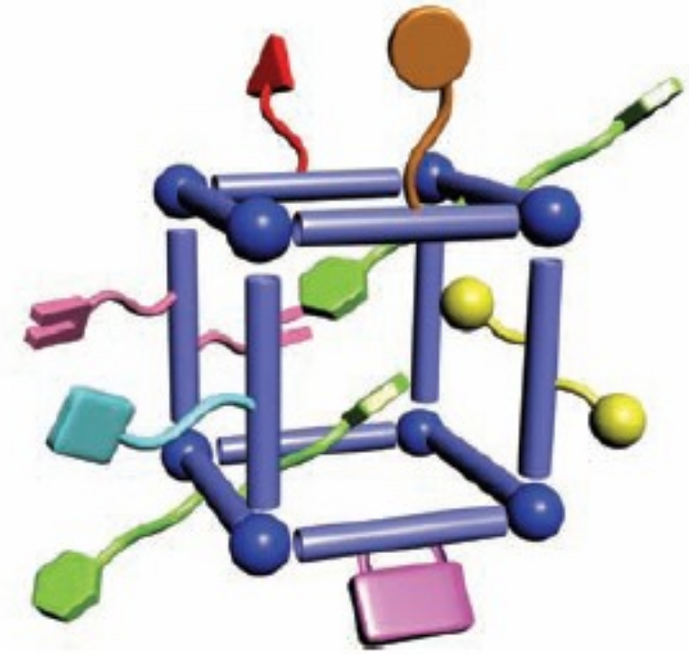

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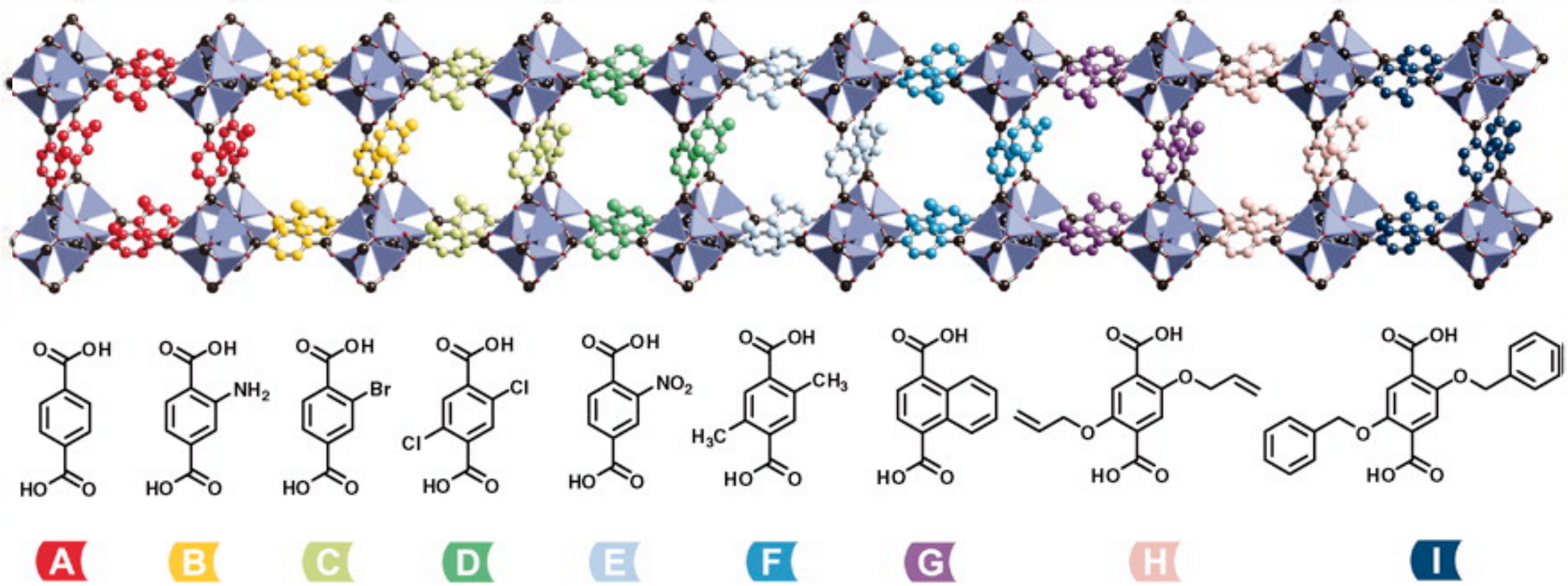

Deng. et al.
Science 2010

- Certain MTV-MOFs have better H_2 and CO_2 adsorption properties than MOFs with a single type of linker.

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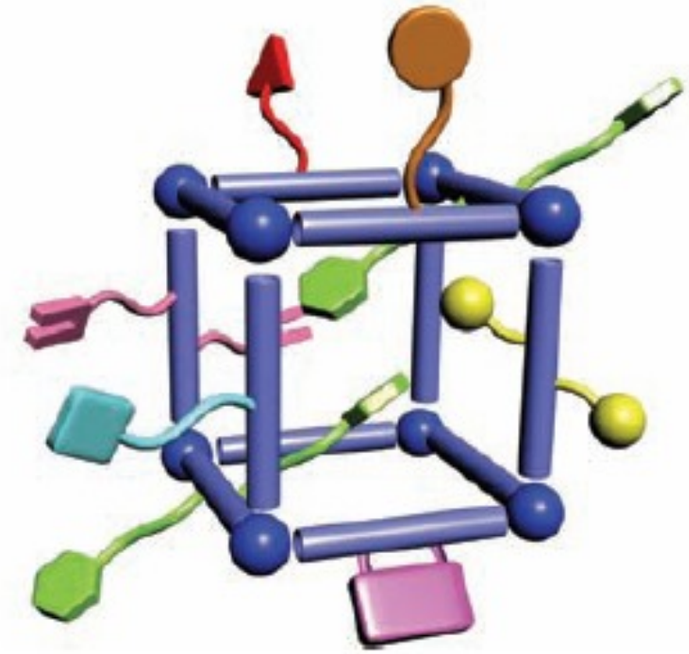

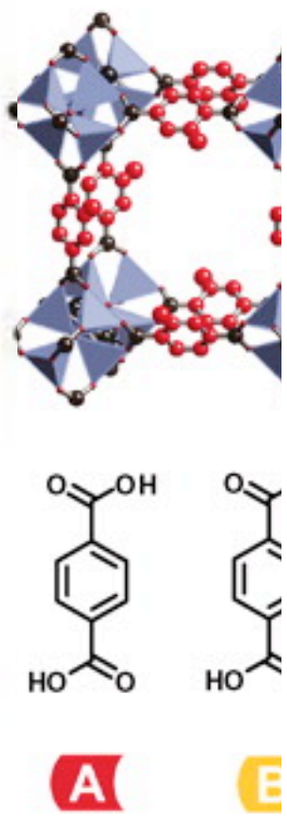

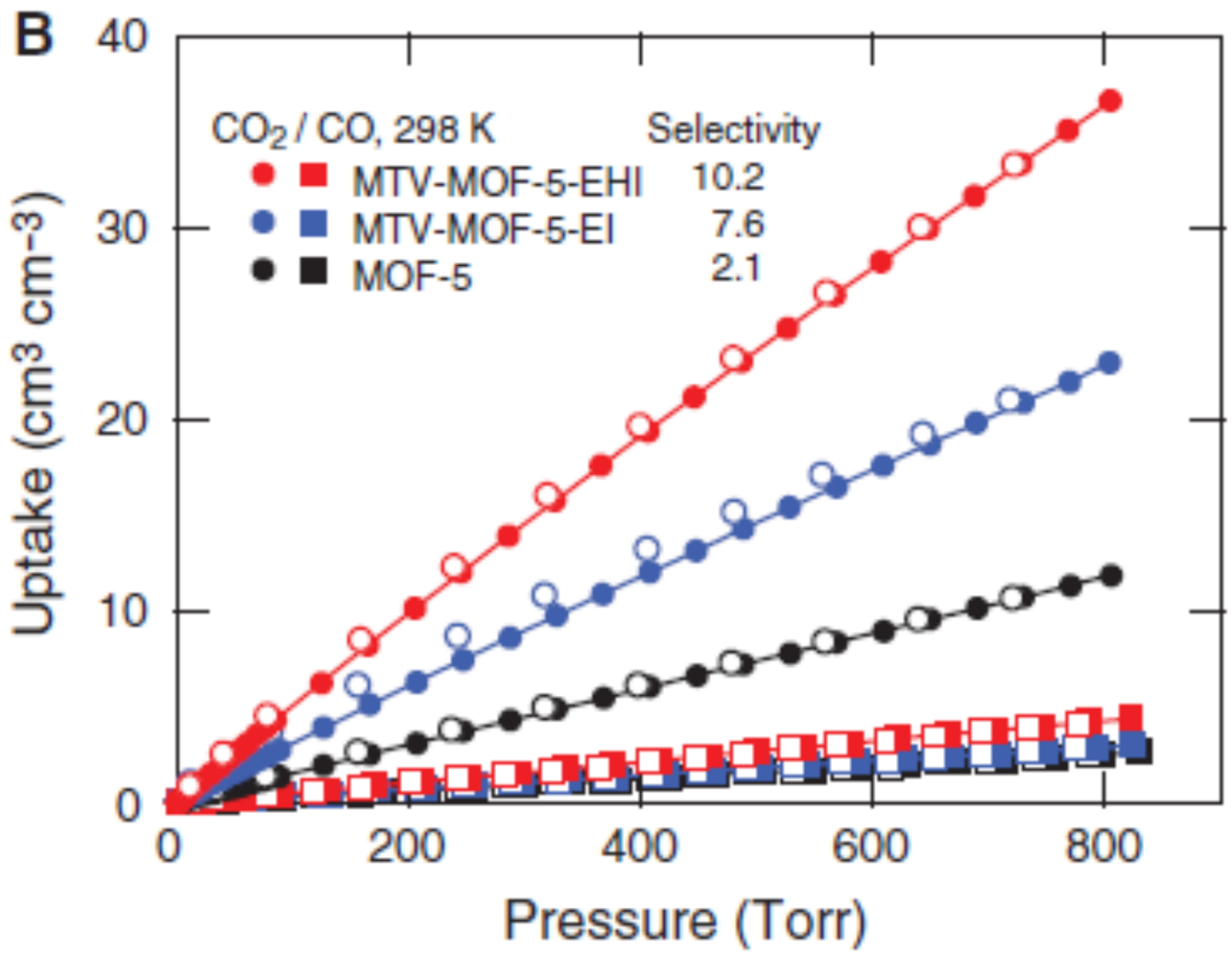

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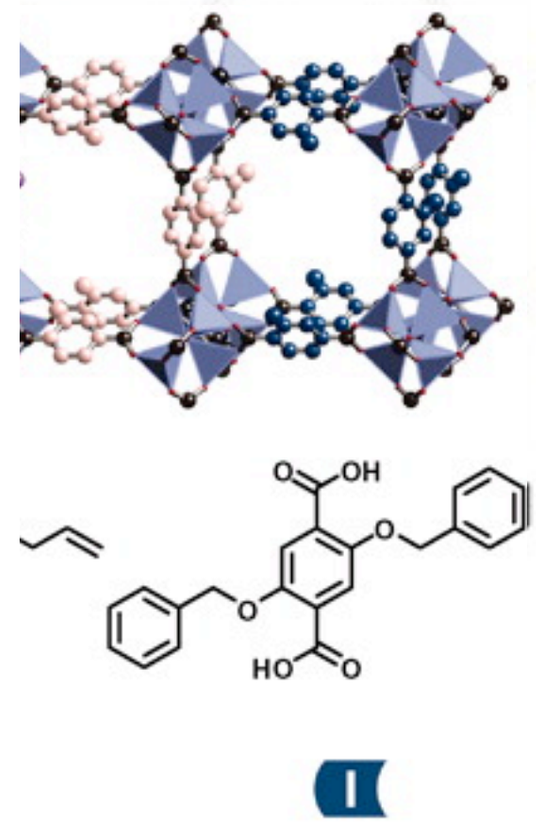

Deng. et al. Science 2010

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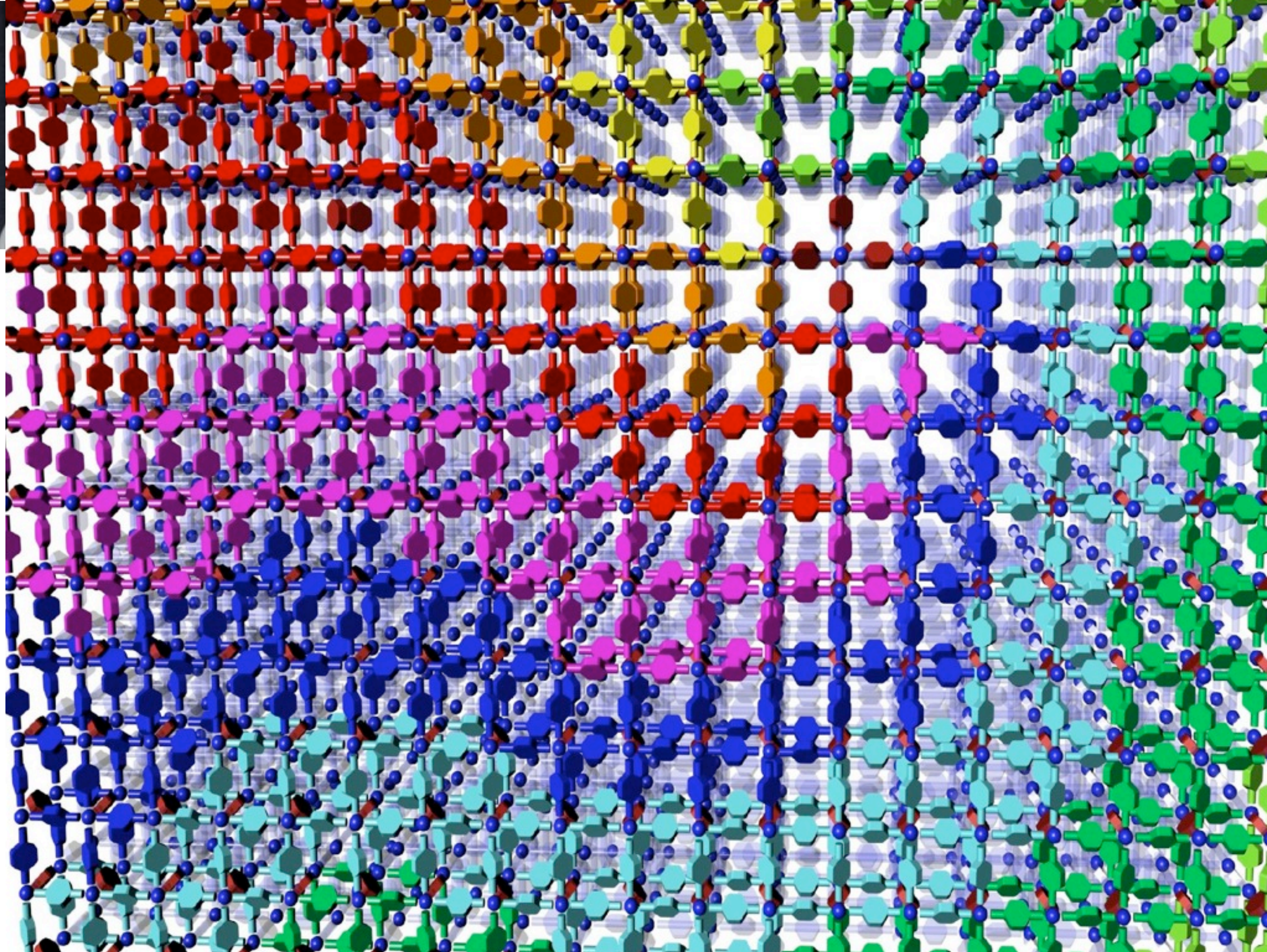
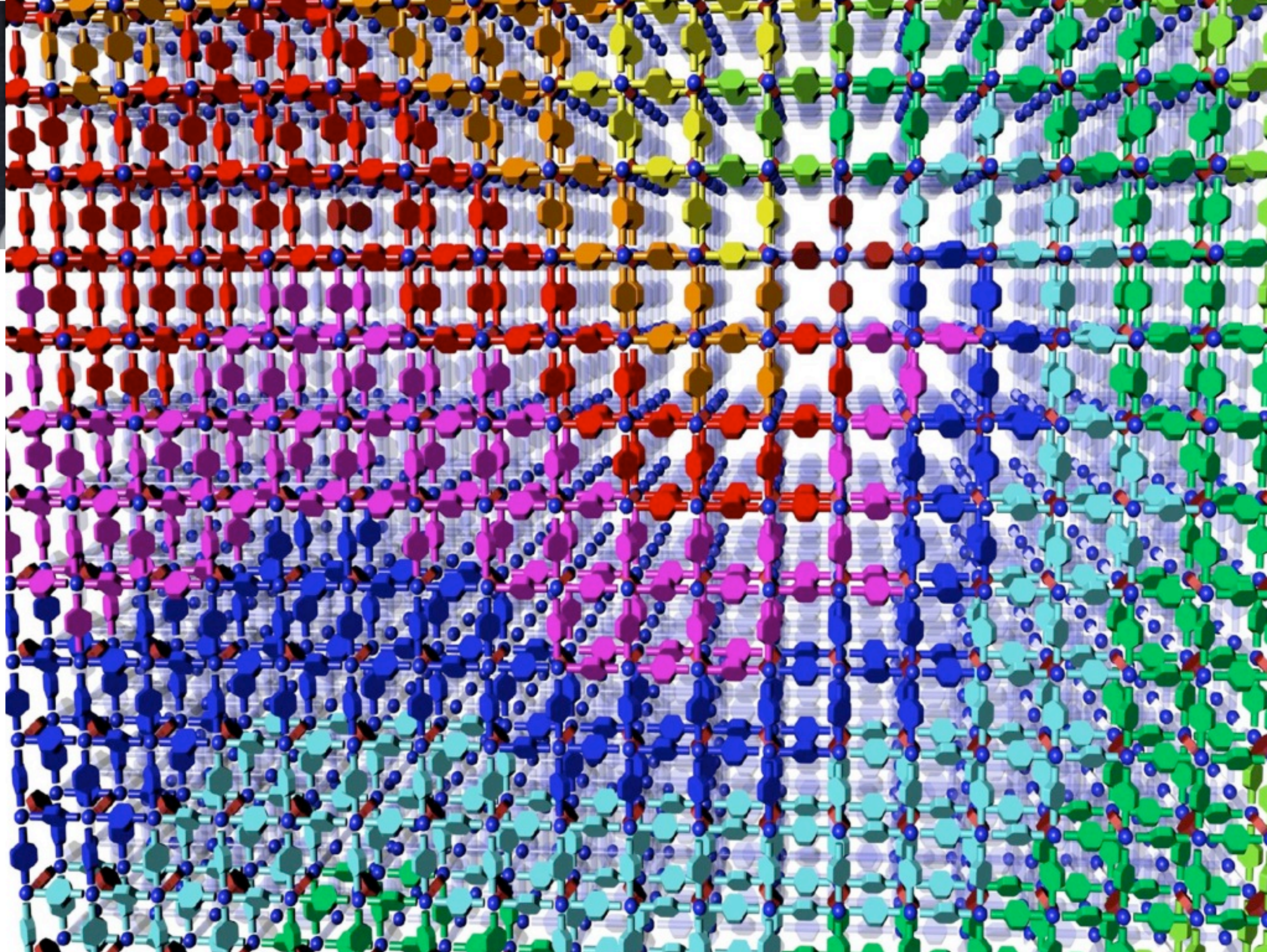
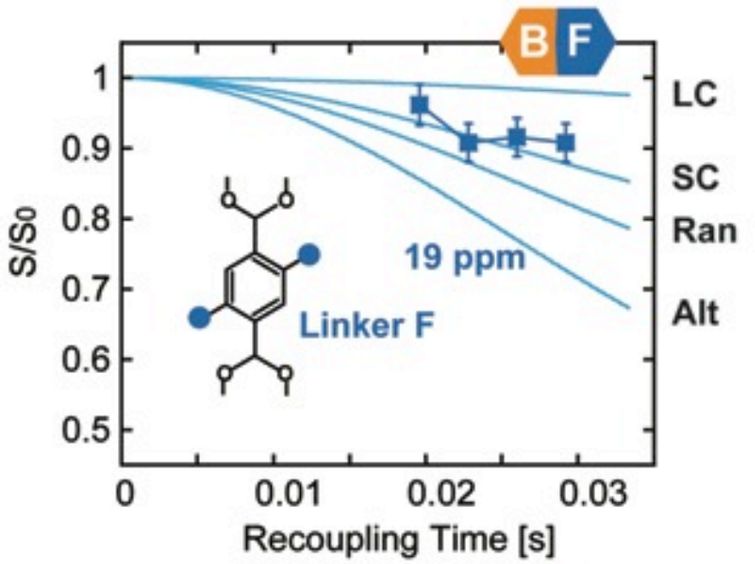
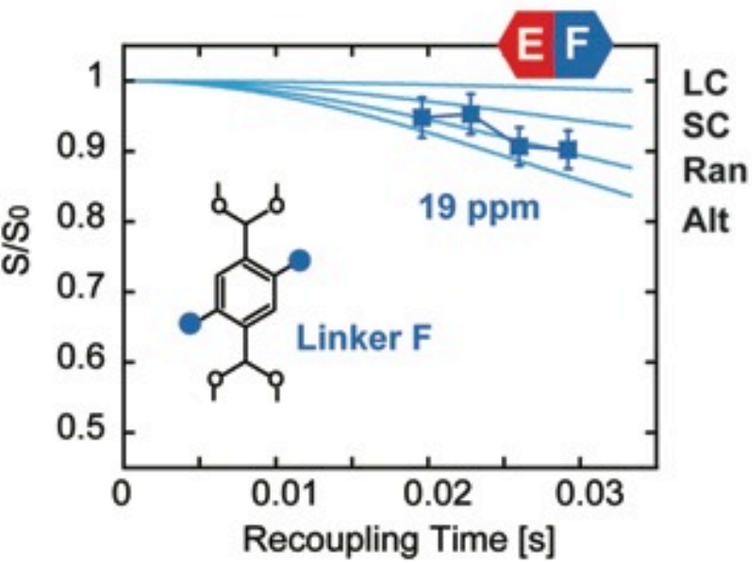
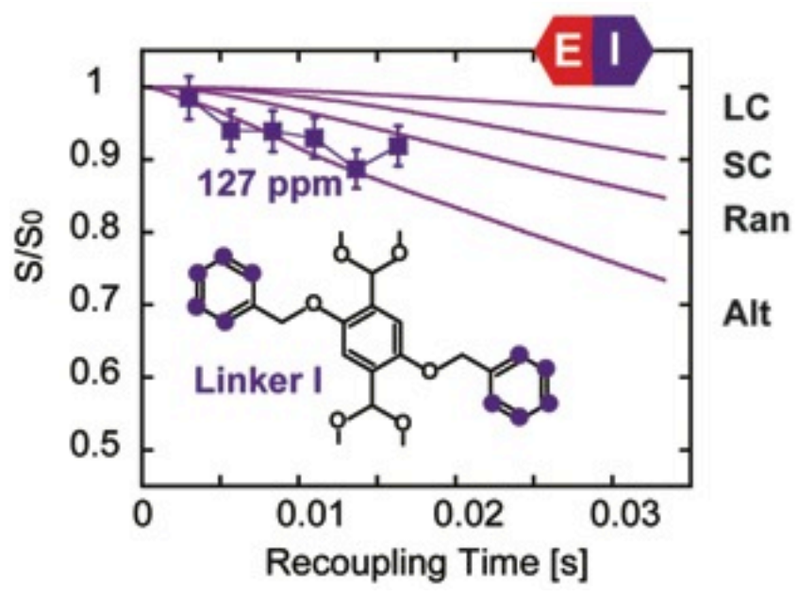




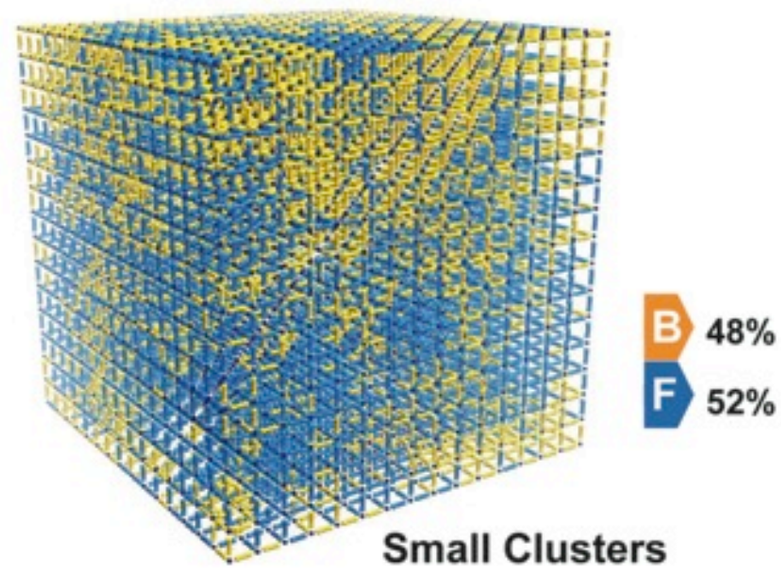
$^{13}C\{^{15}N\}$ REDOR curves

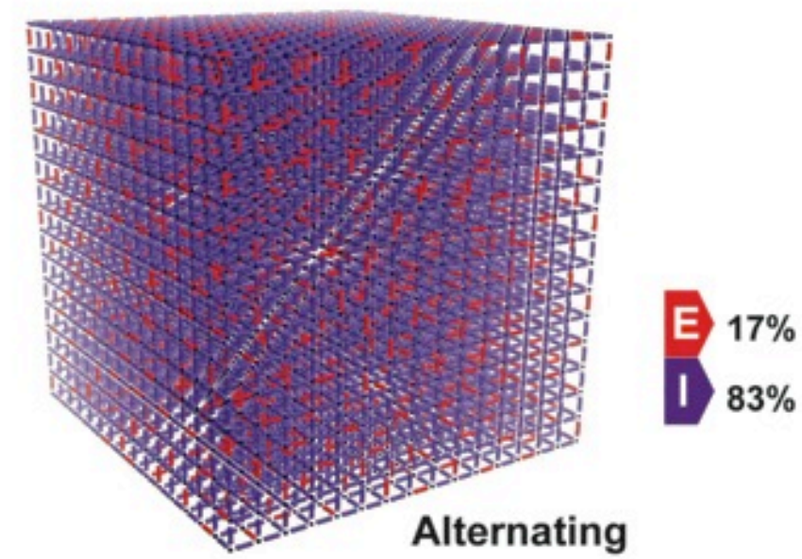


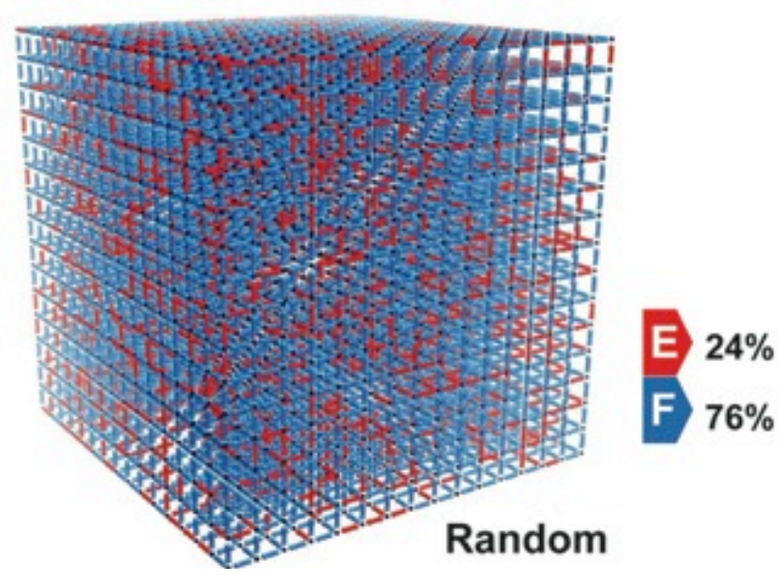


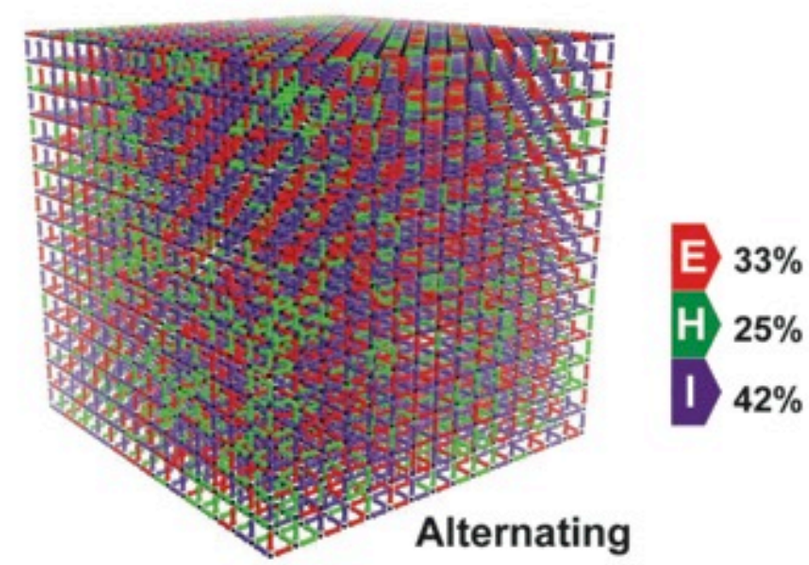


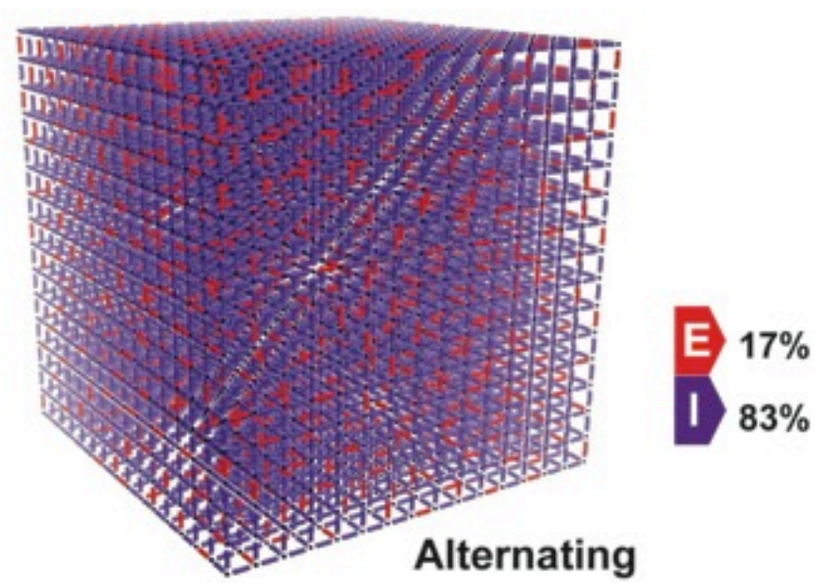
Scenarios of linker apportionment in MTV-MOF-5 materials





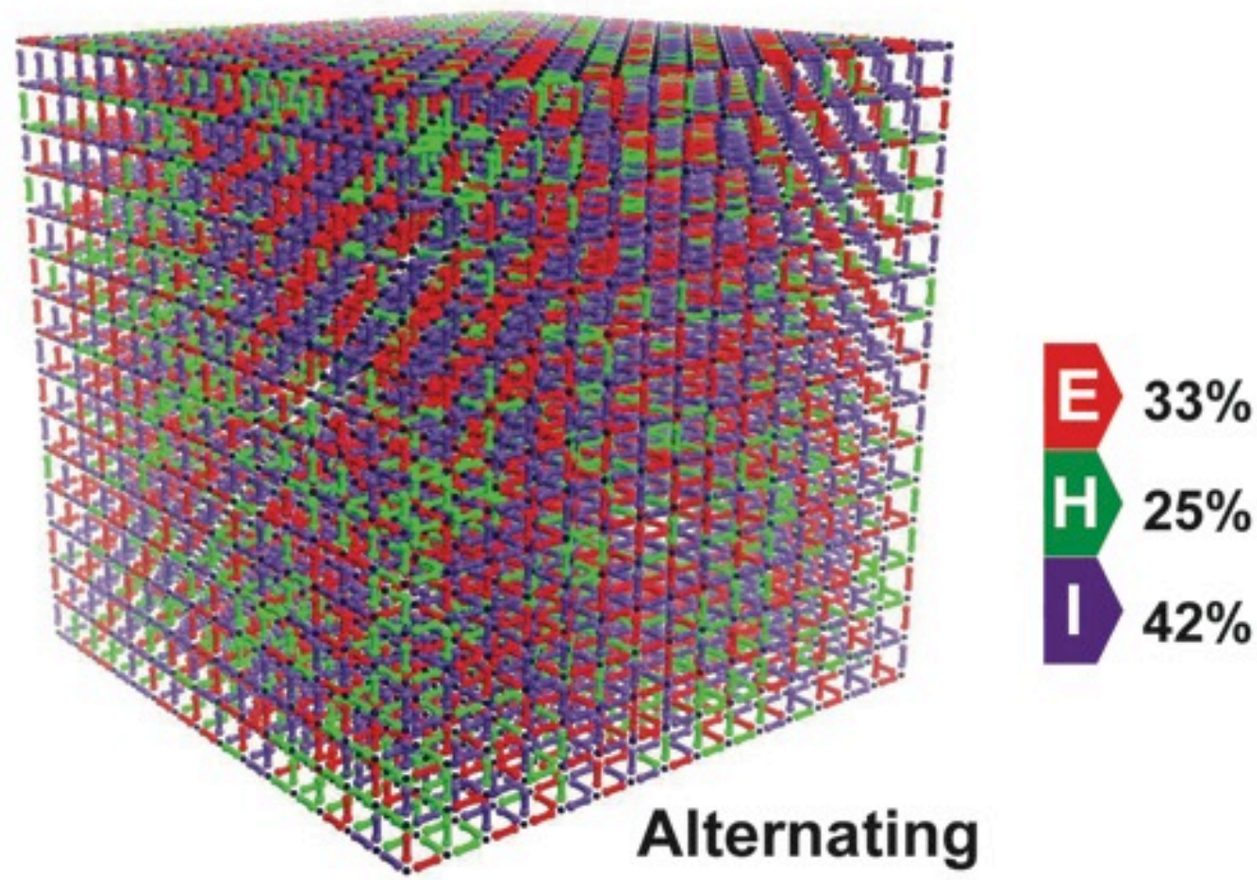






Kong et. al. Science, in press

Apportionment matters



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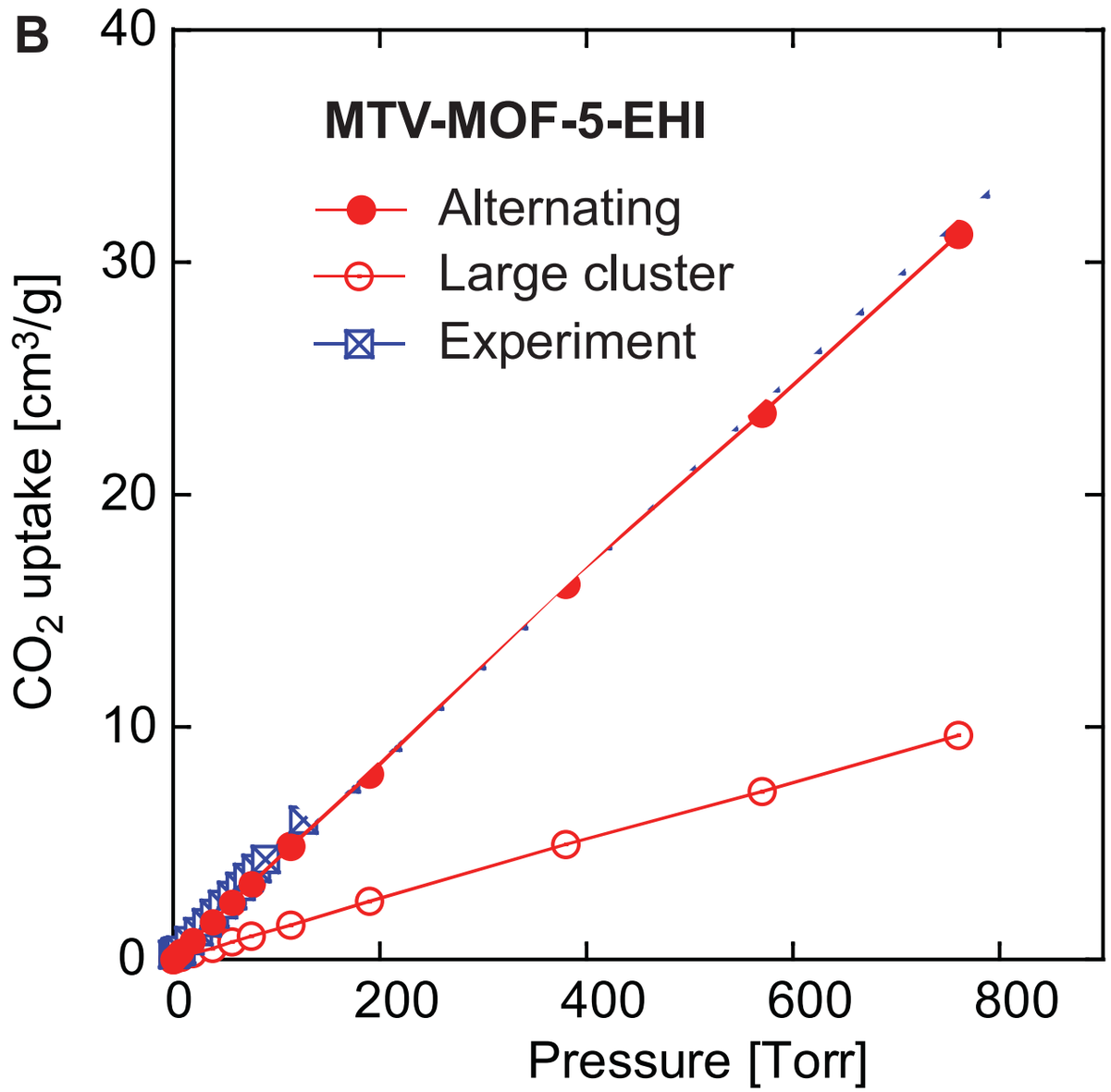

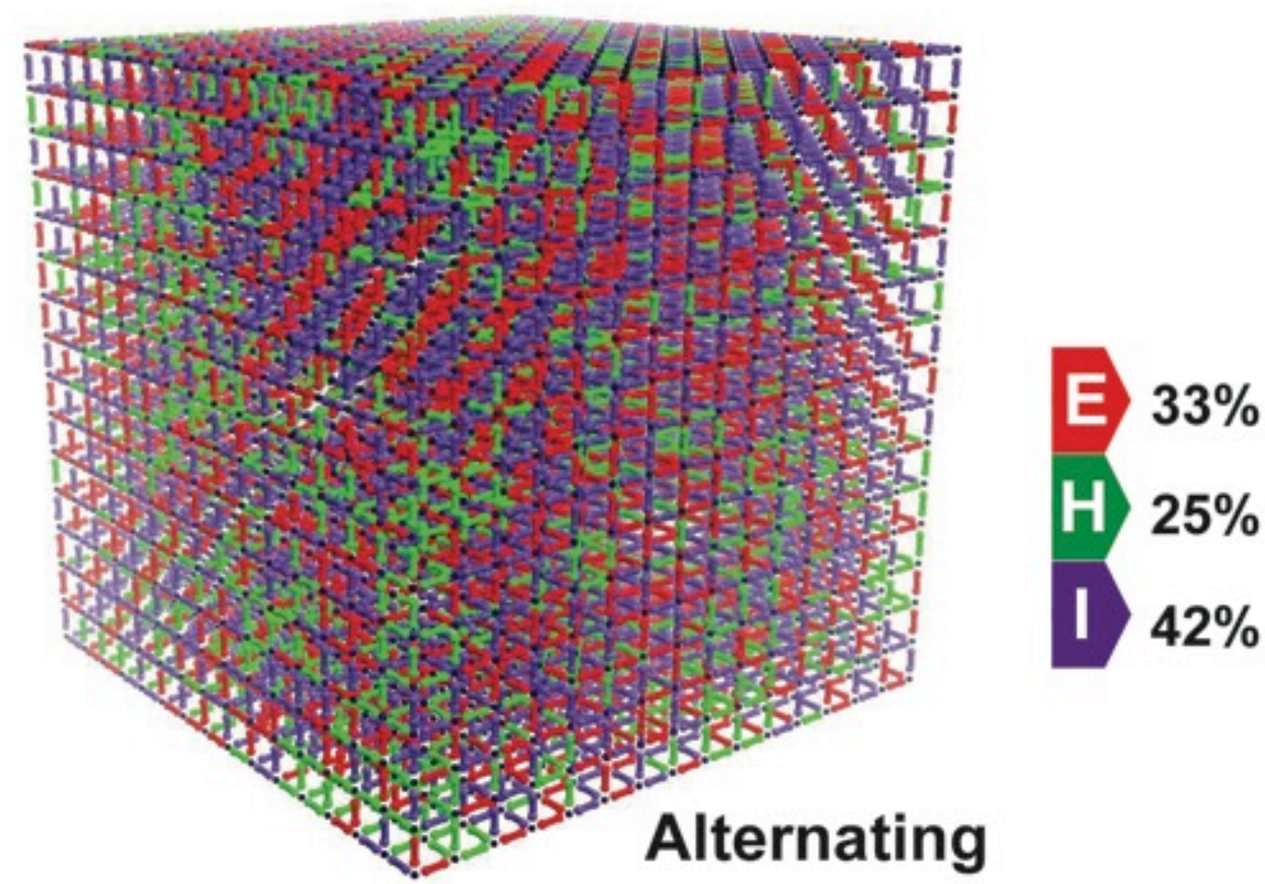

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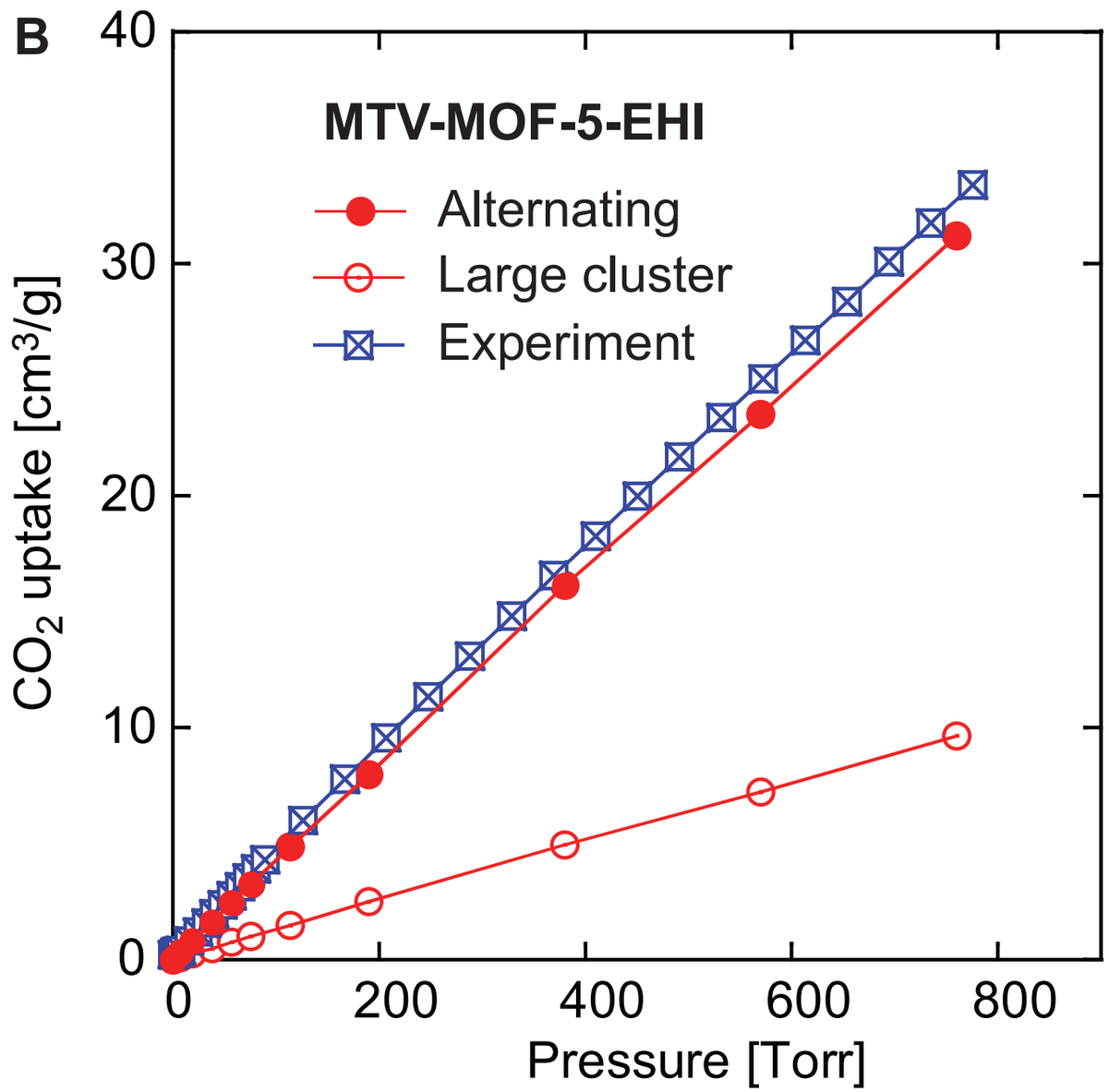

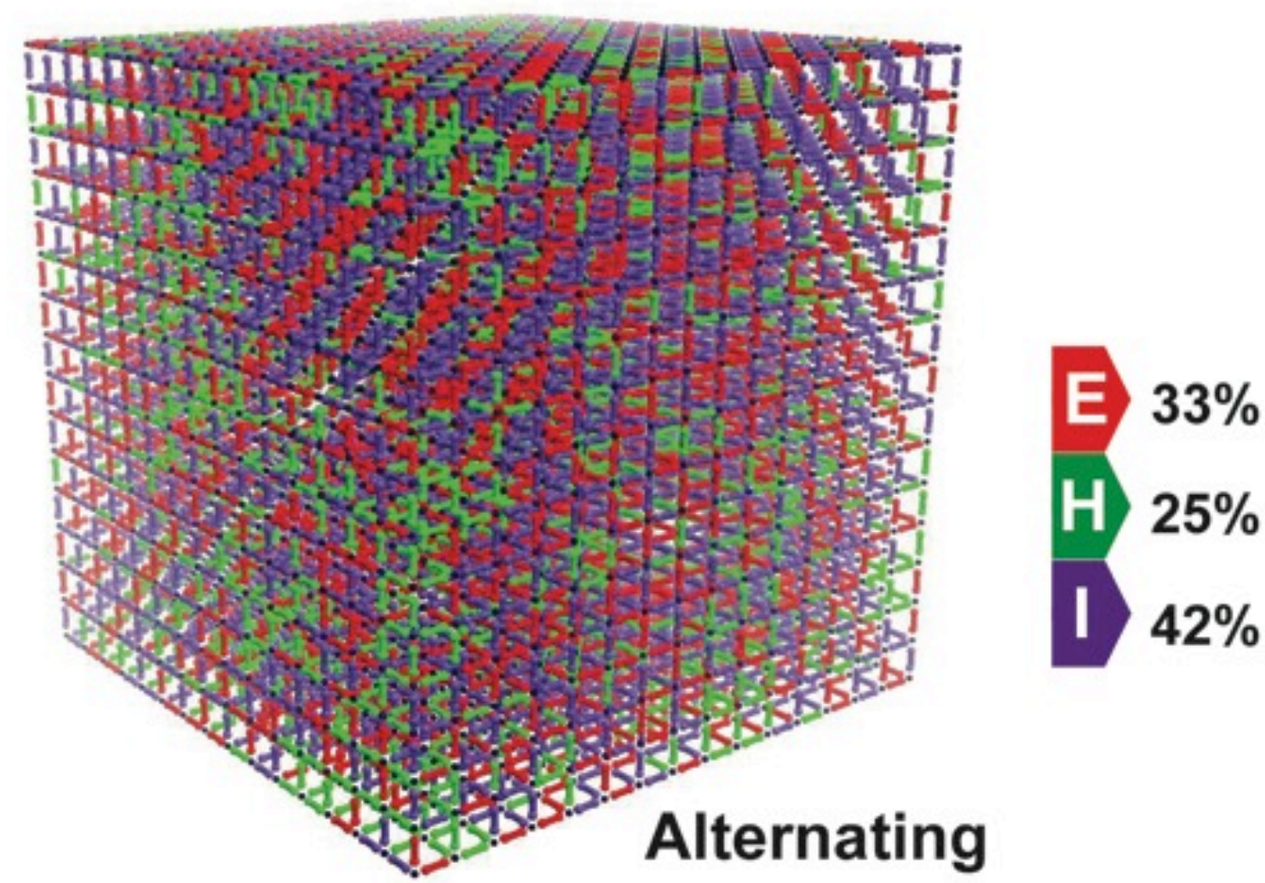

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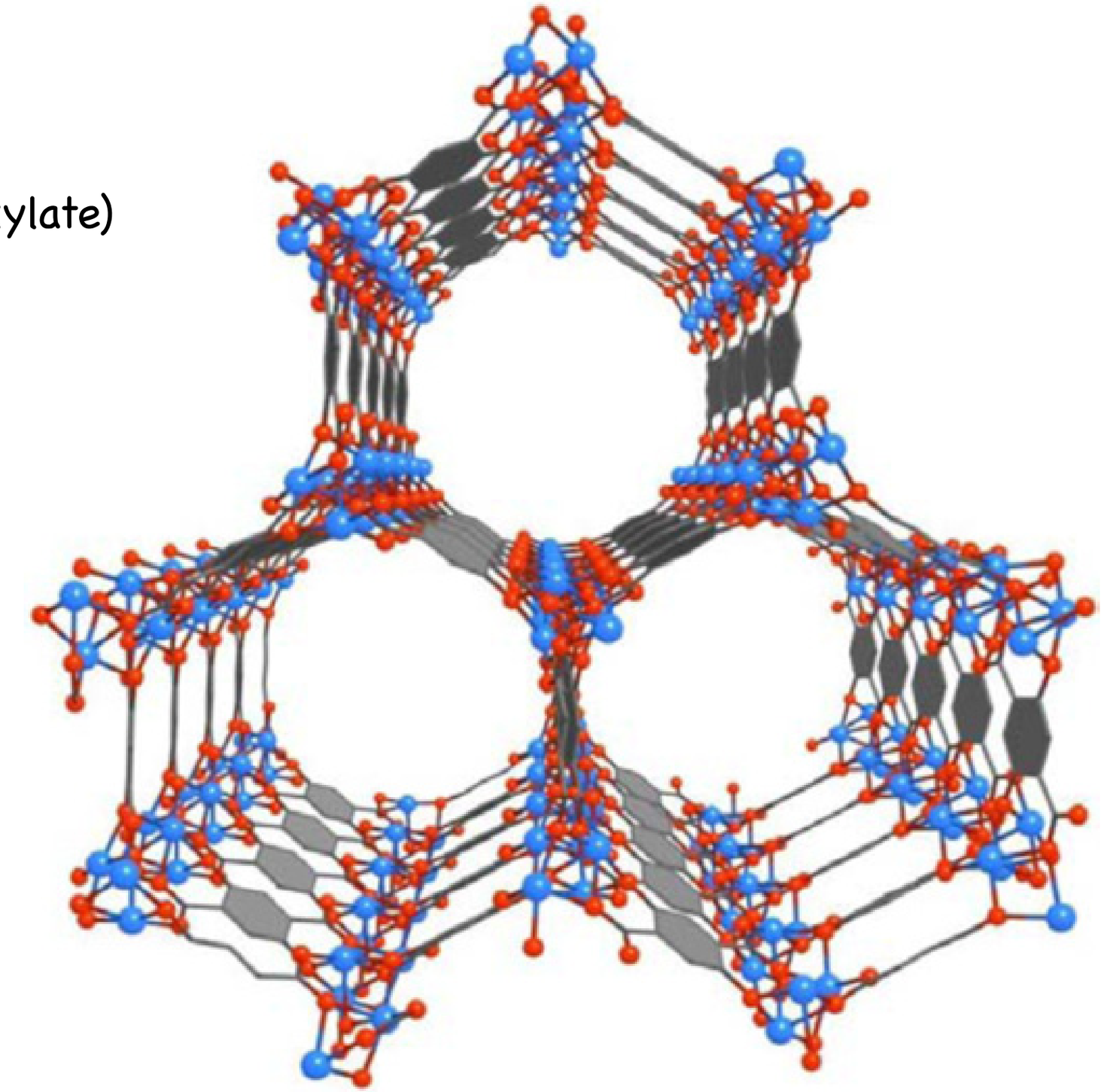
Mg_2(2,5-dioxido-1,4-benzenedicarboxylate)

"Mg-MOF-74"



CO_2 has strong affinity for open metal sites, Mg^{2+}

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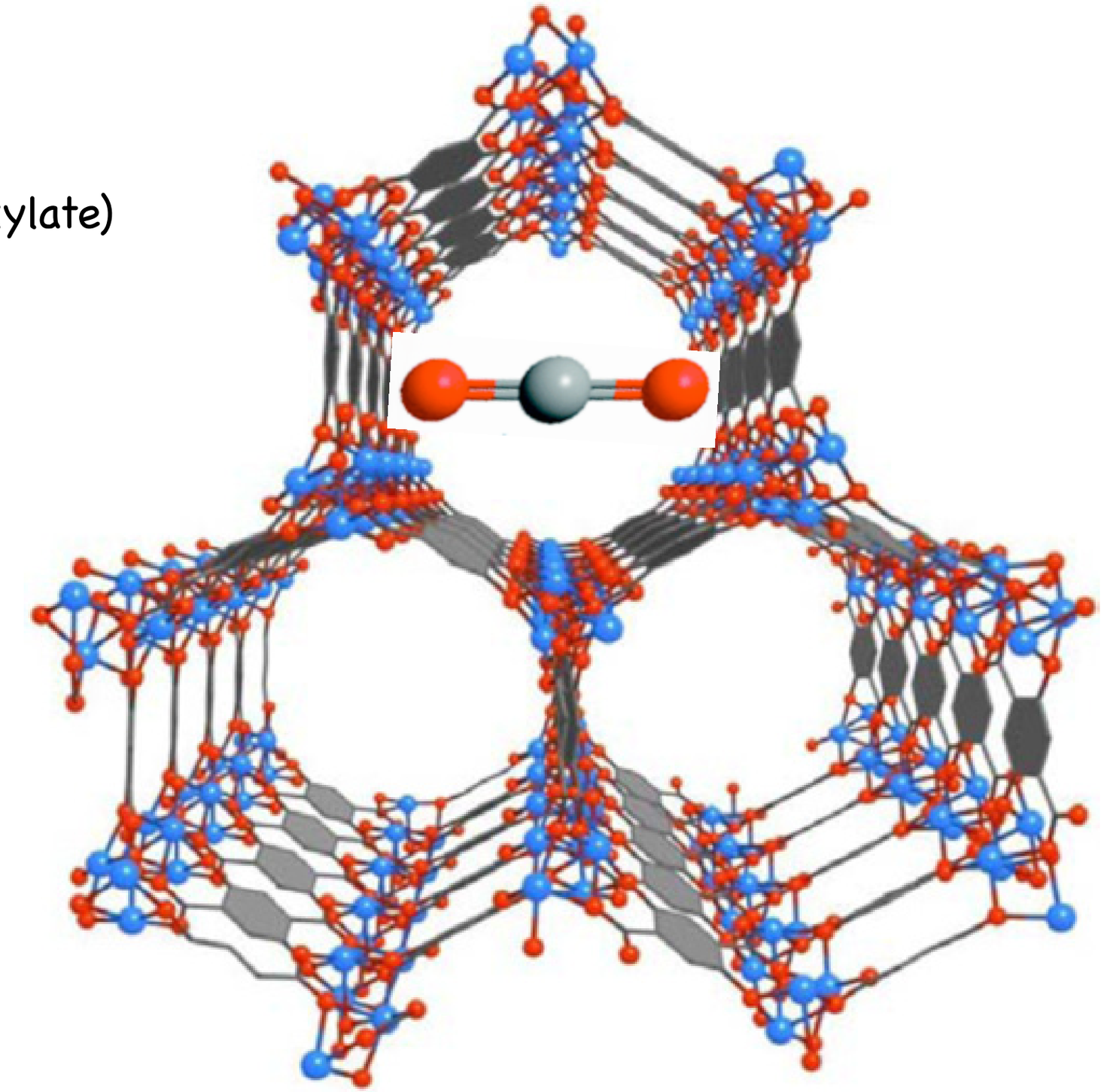

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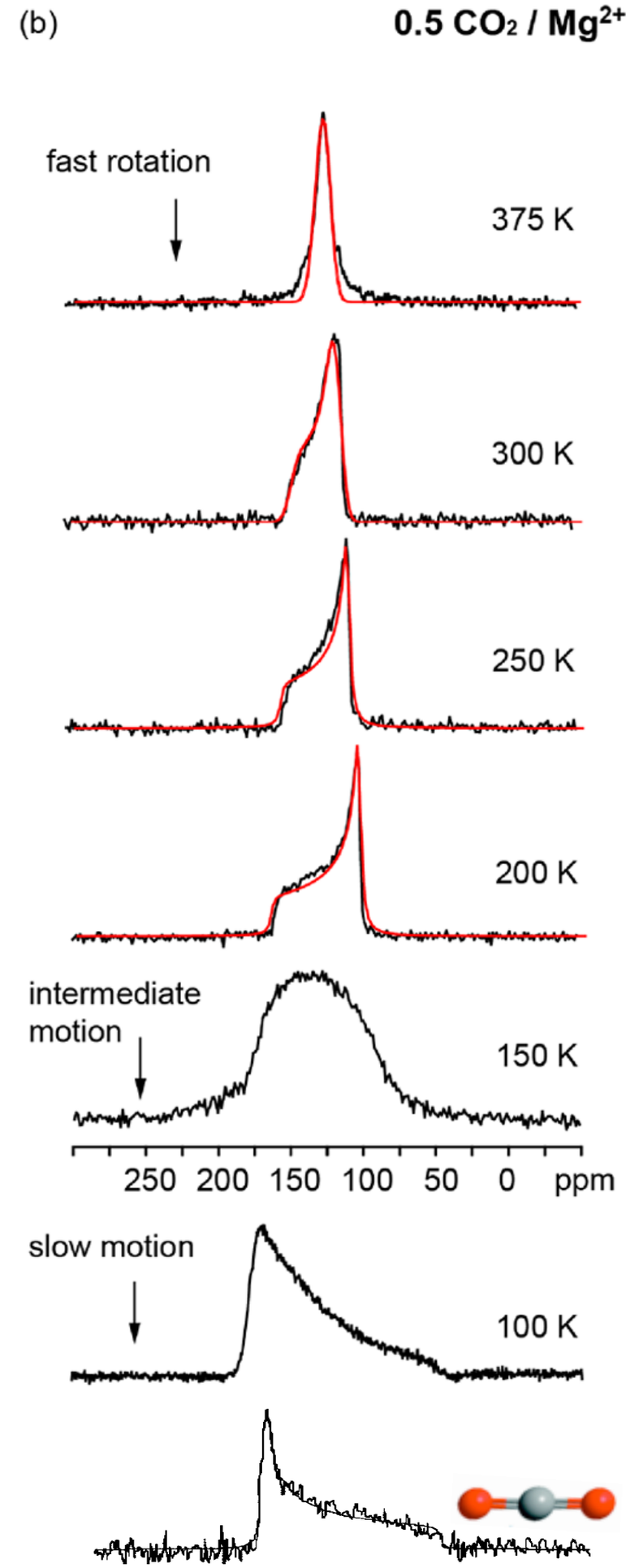
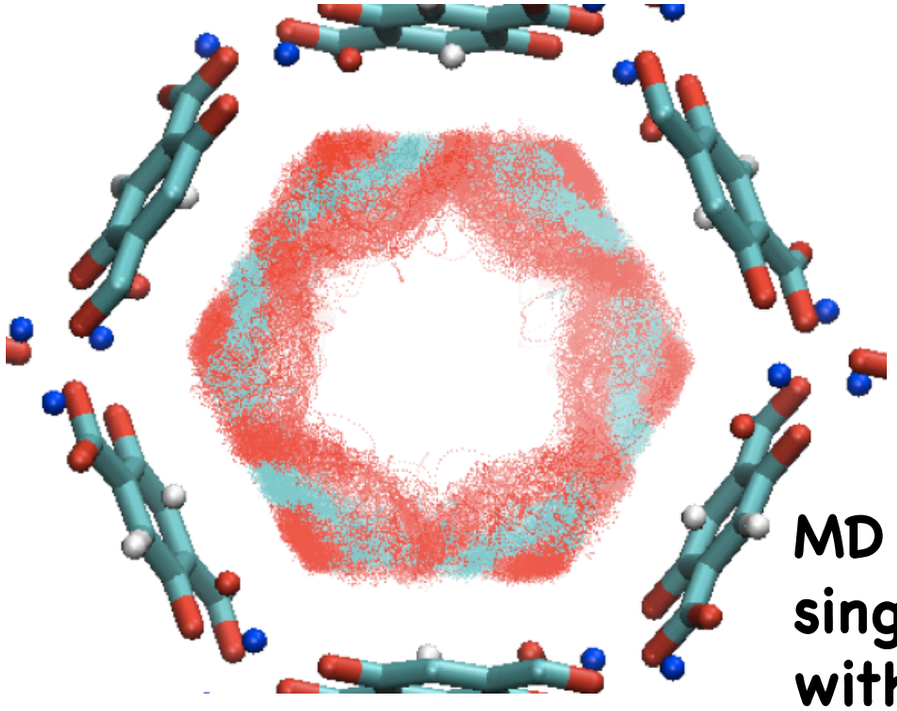
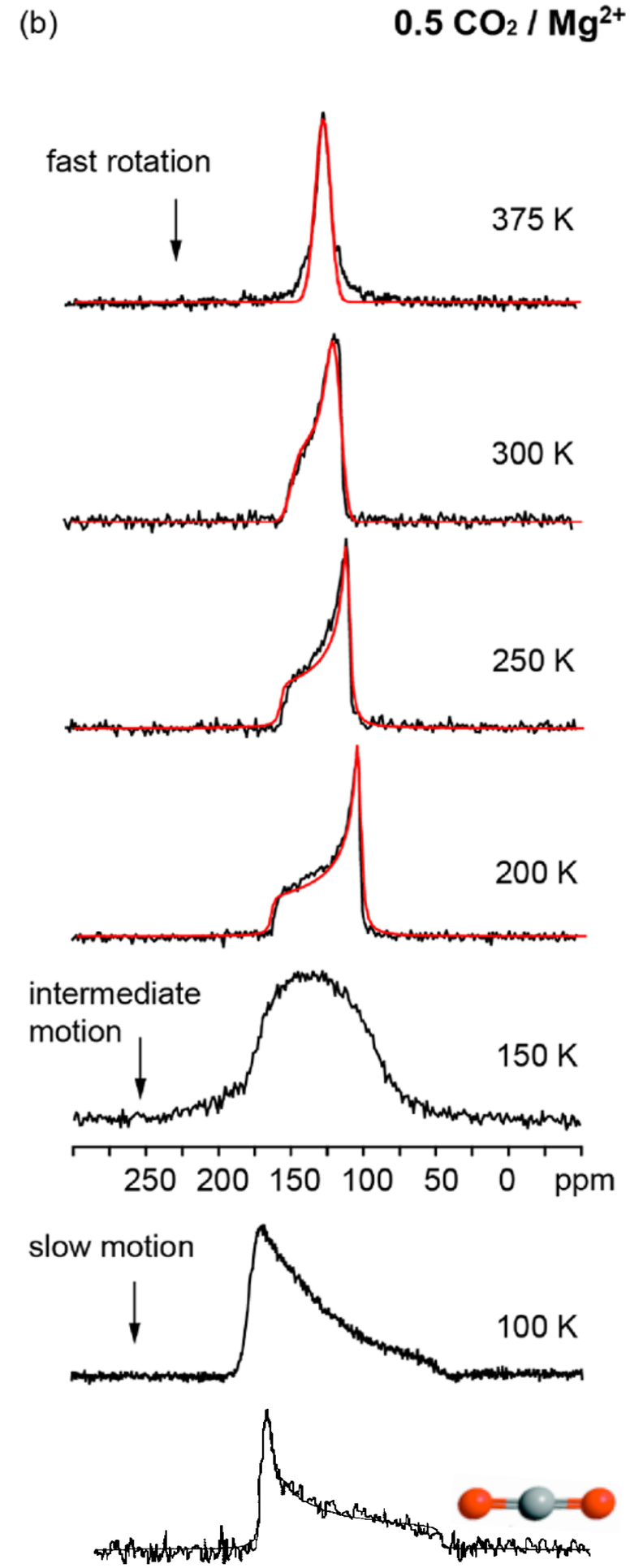


$^{13}CO_2$ NMR in Mg-MOF-74



MD trajectories of a single CO_2 at 200 K with the time period of 5 ns in Mg-MOF-74 structure.



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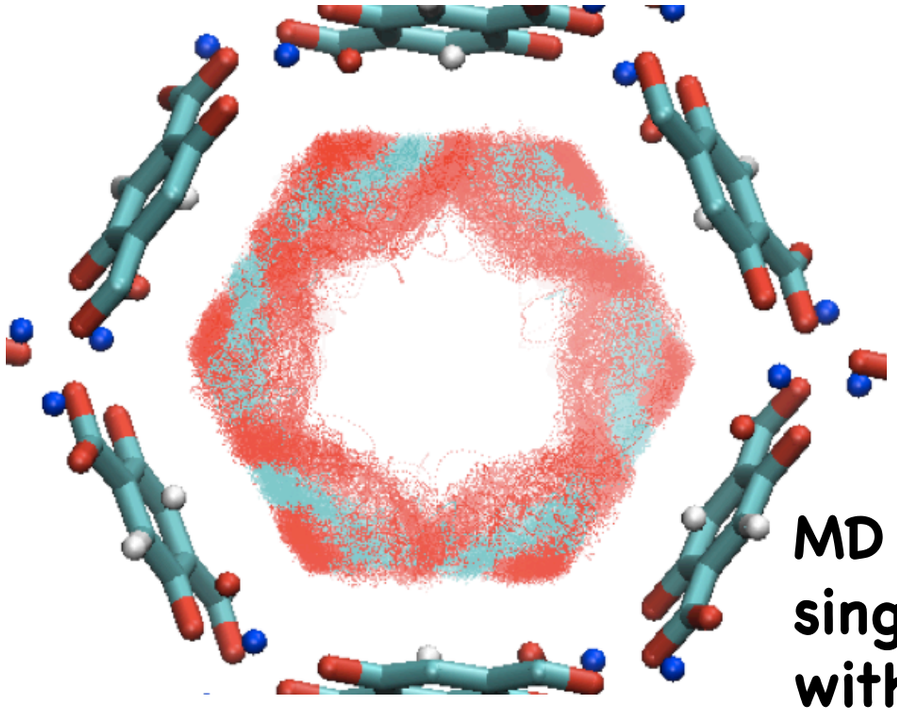

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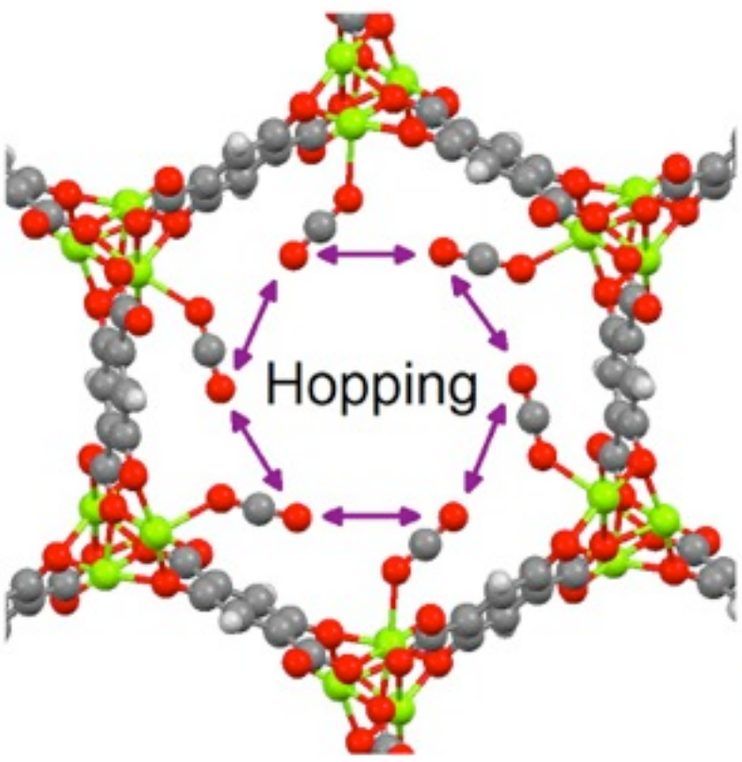
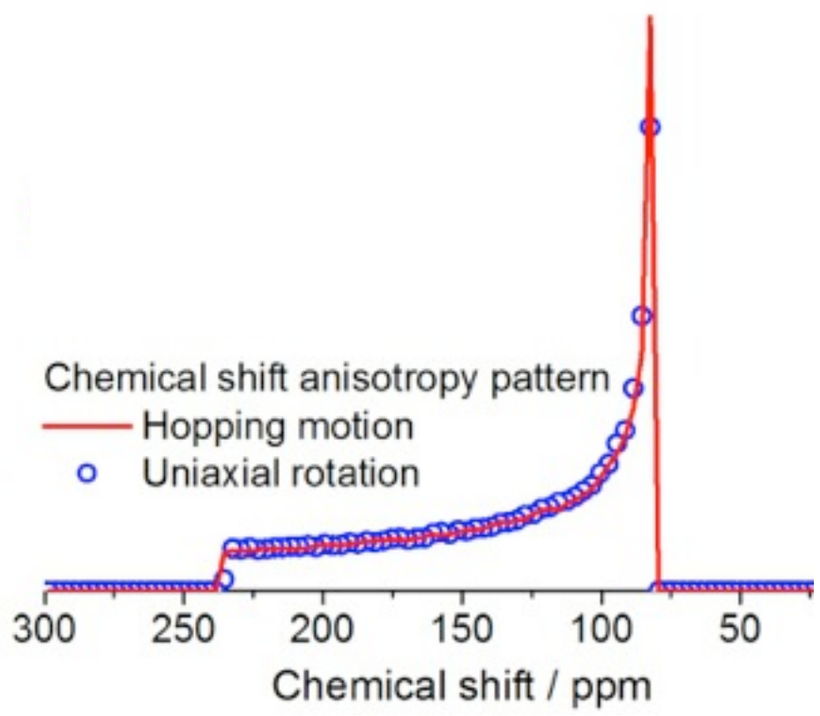
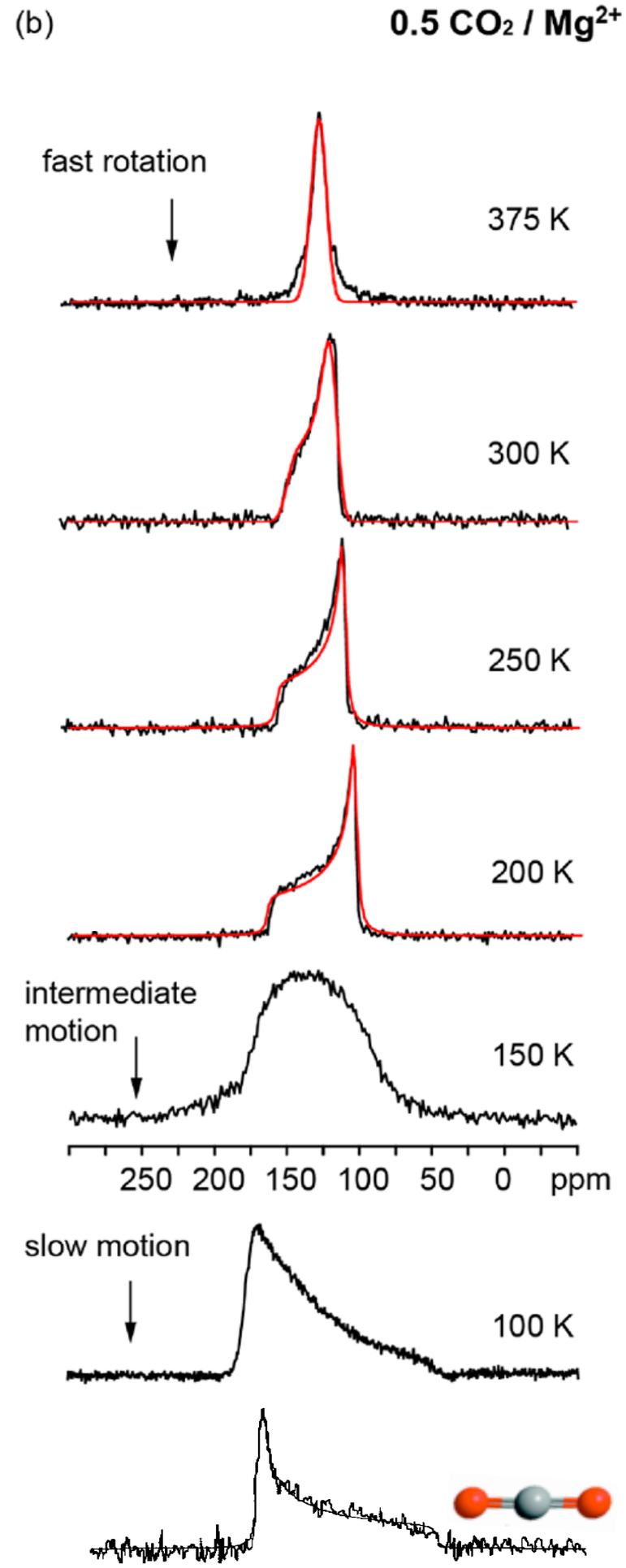






$^{13}CO_2$ NMR in Mg-MOF-74

Berend Smit

Blandine Jerome

Brett Helms

David Luebke

Frantisec Svec

Giulia Galli

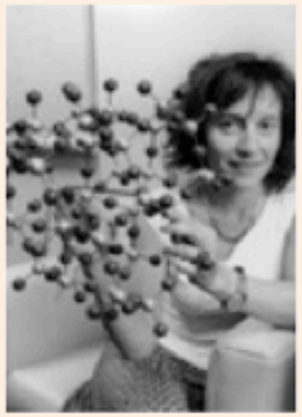
Hongcai (Joe) Zhou

Jeff Kortright

Jeffrey Long

Jeffrey Neaton

Jeffrey Reimer



Laura Gagliardi

Maciej Haranczyk

Omar Yaghi

Simon Teat

Ting Xu

High-Throughput Discovery of Robust Metal-Organic Frameworks for CO_2 Capture

Jeffrey A. Reimer,[4] Tae-Hyun Bae,[1,2] Adam H. Berger,[3] Joseph Chen,[4] Justin J. Dutton,[5] Kuldeep Jariwala,[2] Jihan Kim,[2] Sean Kong,[4] Li-Chiang Lin, Richard L. Martin,[6] Jarad A. Mason,[1] Thomas M. McDonald,[1] Ken J. Micklash,[5] Roger Sathre,[7] Kenji Sumida,[1] Joseph A. Swisher,[2,4] Abhoyjit S. Bhown,[3] Maciej Haranczyk,[6] Steven Kaye,[5] Jeffrey R. Long,[1,2] Eric Masanet,[7] Berend Smit [1,2,4]

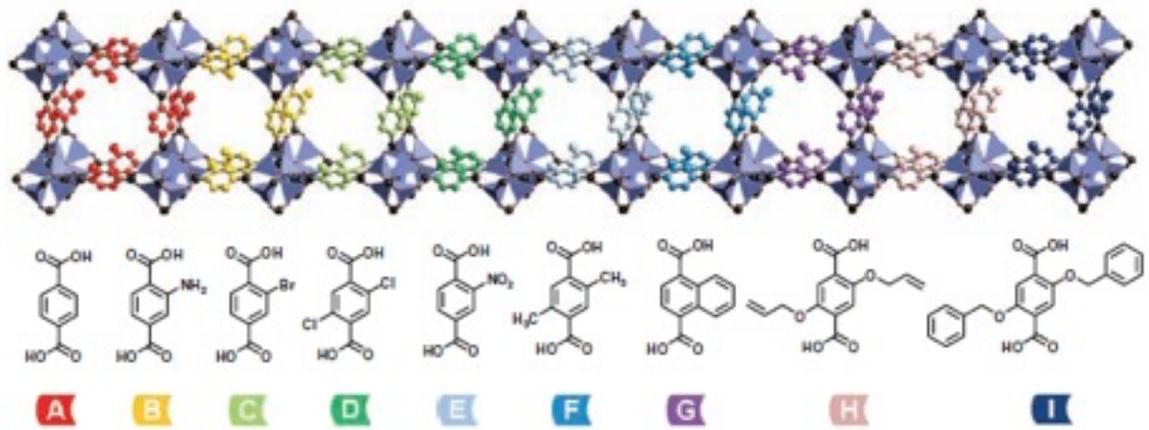
[1]Department of Chemistry, University of California Berkeley, [2]Materials Sciences Division, Lawrence Berkeley National Laboratory, [3]Electric Power Research Institute (EPRI), [4]Department of Chemical and Biomolecular Engineering, University of California Berkeley, [5]Wildcat Discovery Technologies Inc., [6]Computational Research Division, Lawrence Berkeley National Laboratory, [7]Environmental Energy Technologies Division, Lawrence Berkeley National Laboratory

Tuesday, July 9, 2013 - Grand Station I & II

5:00 p.m. **Poster Session/Reception – Grand Station III**

a dizzying array of possibilities...

MTV-MOF-5 structure
with eight different functionalities



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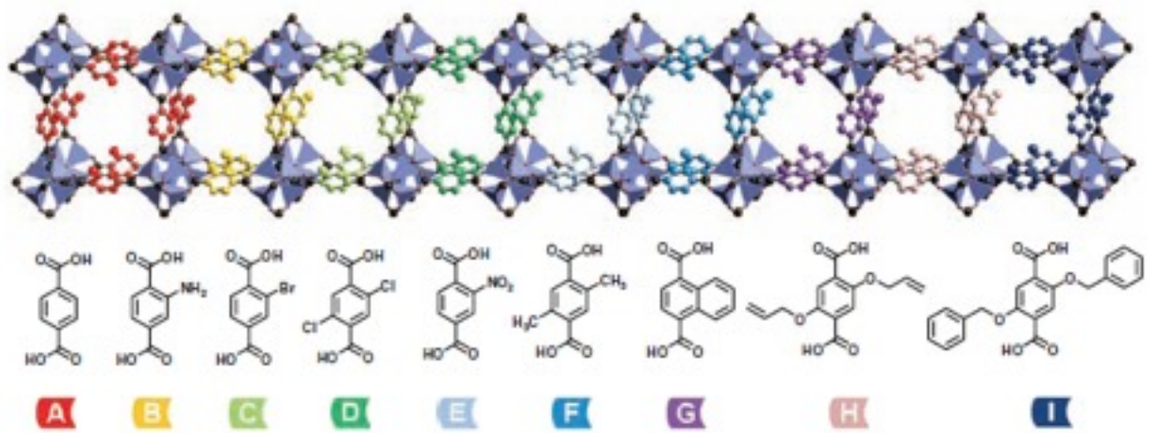

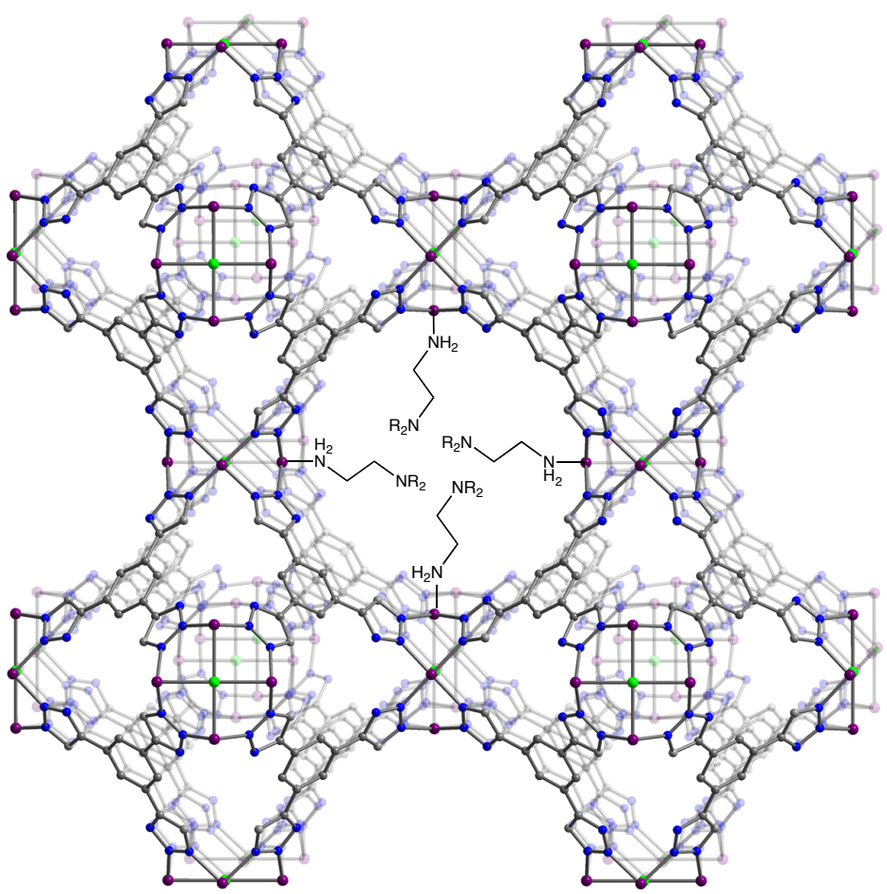

$Cu_3[(Cu_4Cl)_3(BTTri)_8]_2 \cdot xH_2NCH_2CH_2NR_2$

a dizzying array of possibilities...

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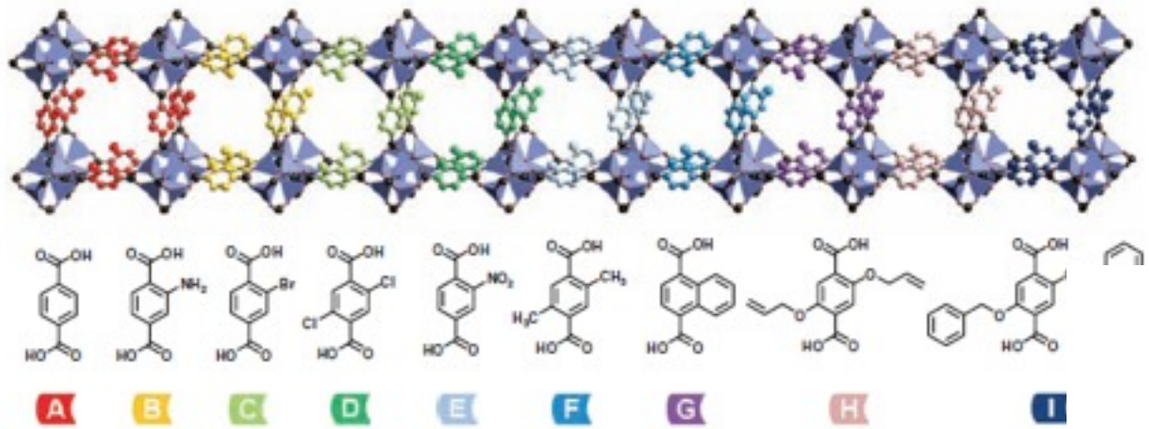
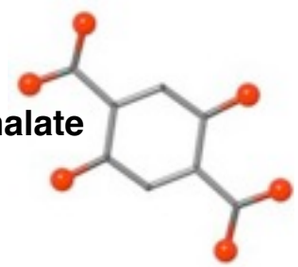
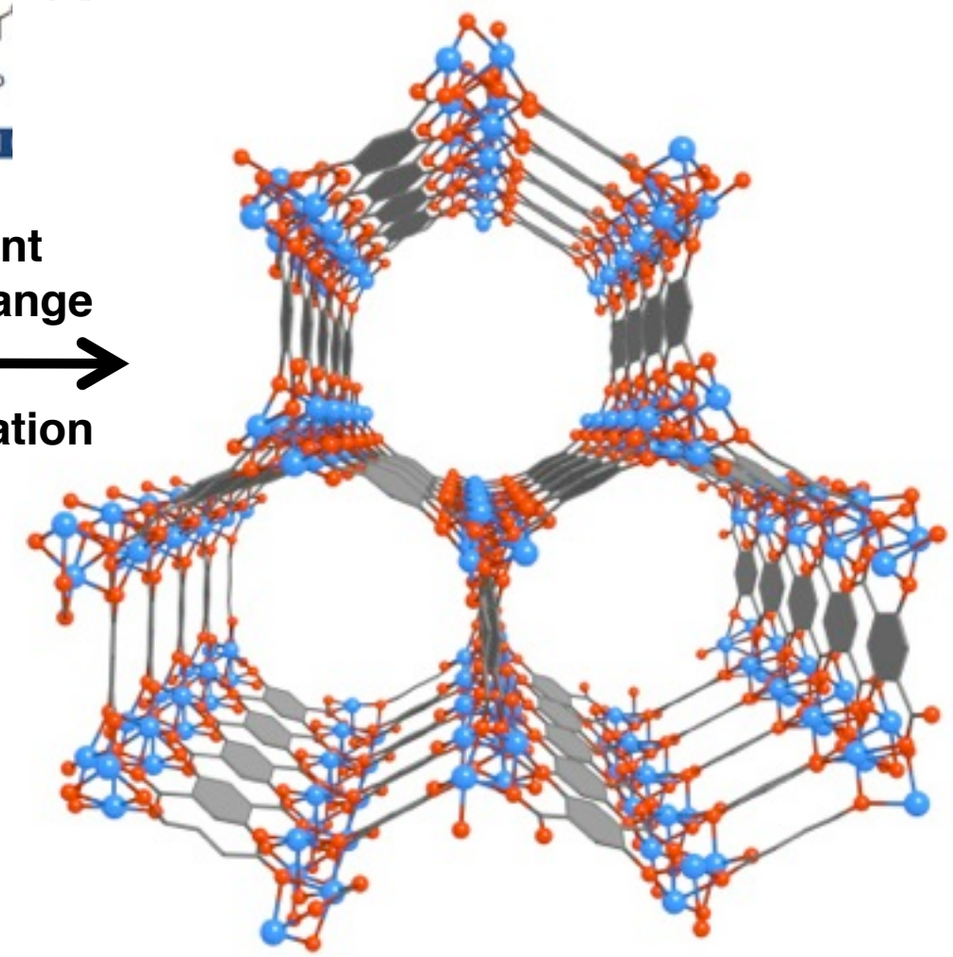


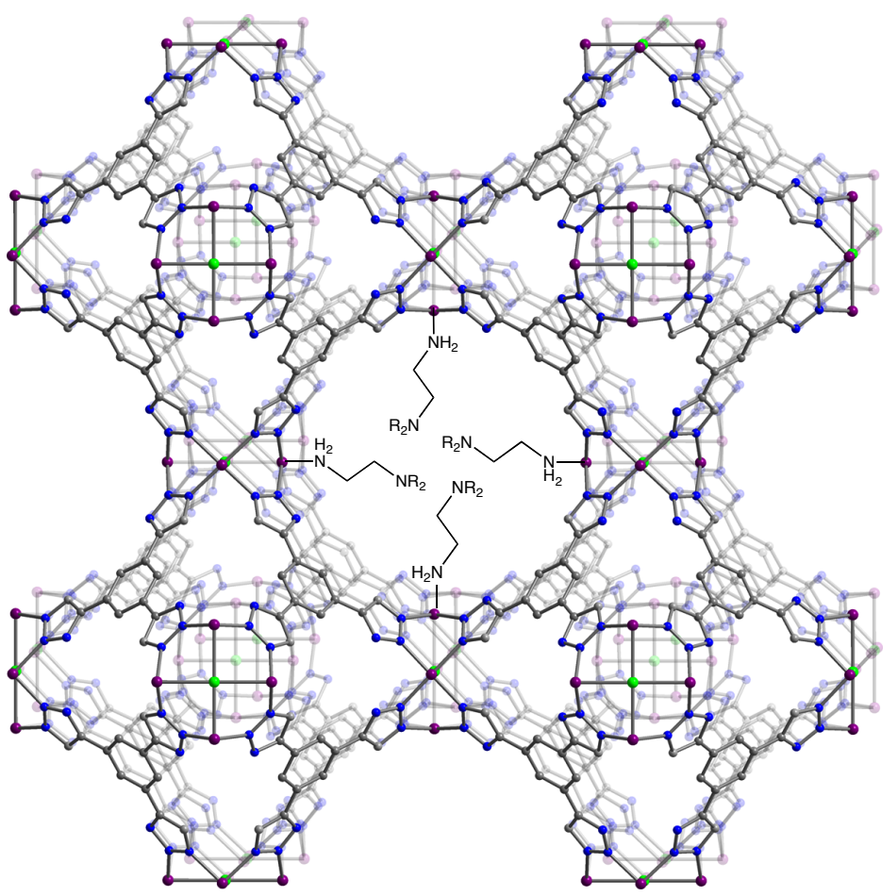
2,5-dioxidoterephthalate
($DOBDC^{4-}$)



+ $M(NO_3)_2 \cdot 6H_2O$ → solvent exchange → activation

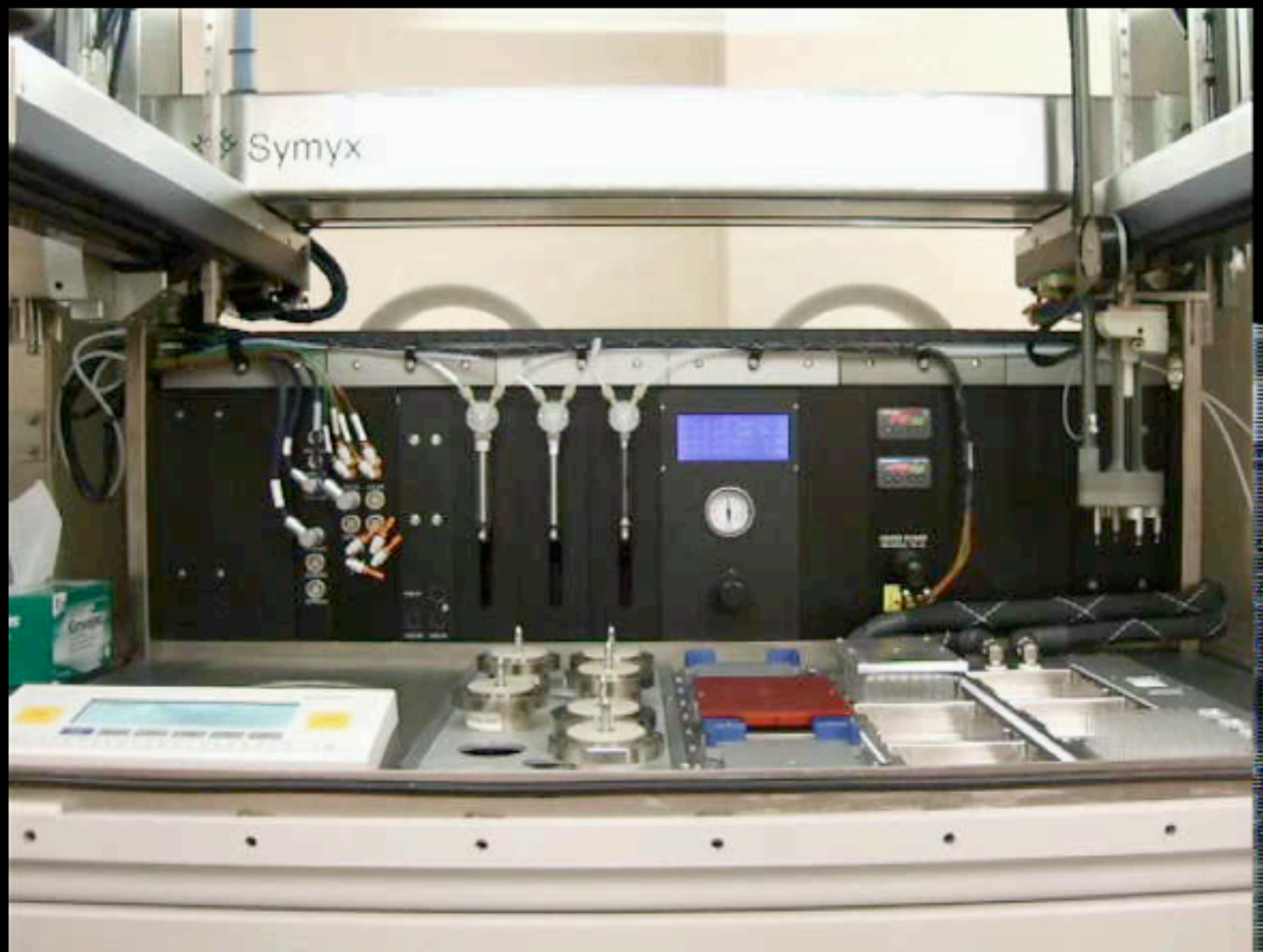


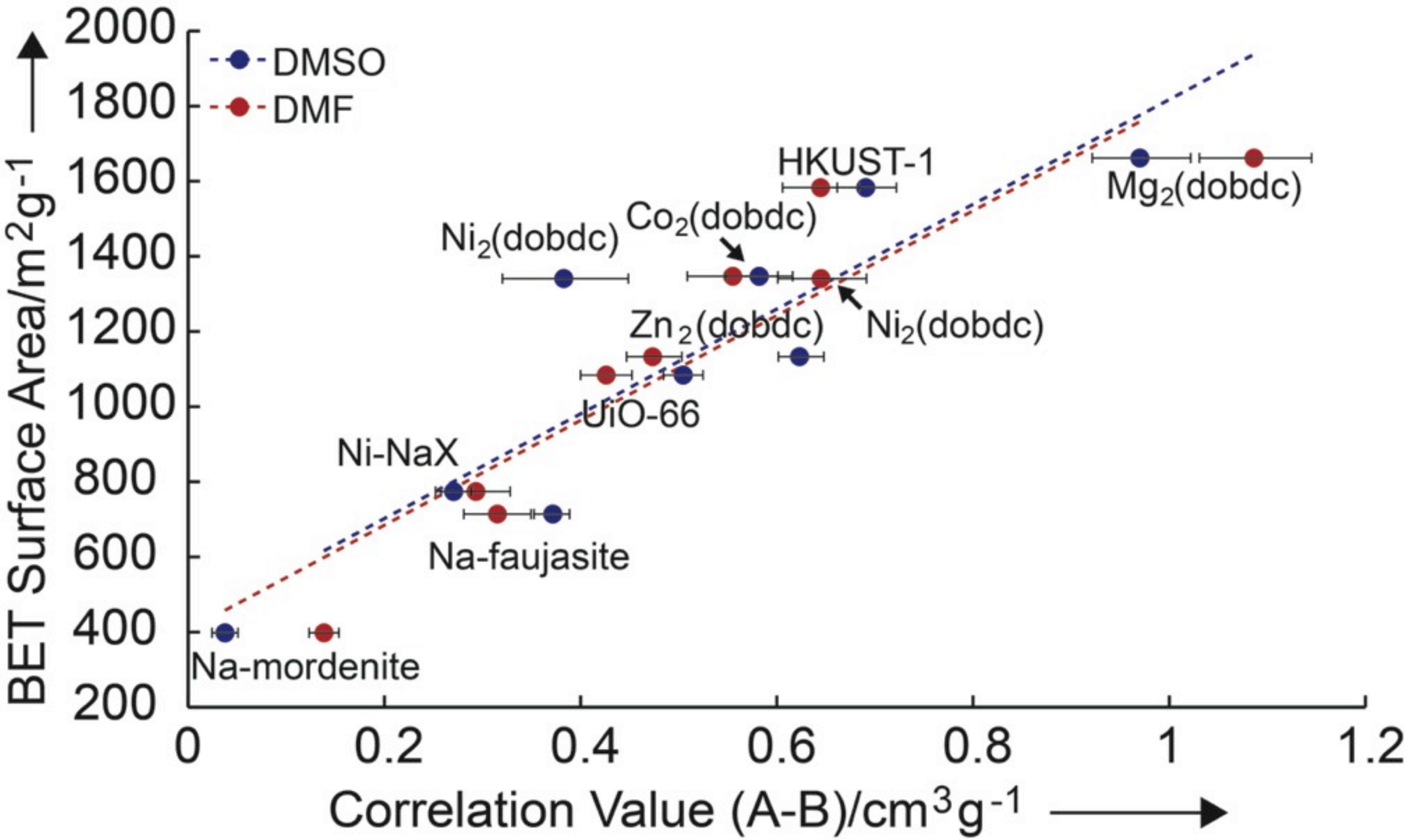
$M_2(DOBDC)$ (M-MOF-74)
(M = Mg, Co, Ni, Zn)



$Cu_3[(Cu_4Cl)_3(BTTri)_8]_2 \cdot xH_2NCH_2CH_2NR_2$

Symyx


Symyx


DMSO
DMF
HKUST-1
Mg2(dobdc)
Co2(dobdc)
Ni2(dobdc)
Zn2(dobdc)
Ni2(dobdc)
UiO-66
Ni-NaX
Na-faujasite
Na-mordenite
BET Surface Area/m2g-1
Correlation Value (A-B)/cm3g-1
2000
1800
1600
1400
1200
1000
800
600
400
200
0
0.2
0.4
0.6
0.8
1
1.2